2006 Lecture Notes on Hilbert Spaces and Quantum Mechanics

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Chapter I

Historical notes and overview

I.1 Introduction

The concept of a Hilbert space is seemingly technical and special. For example, the reader has probably heard of the space ℓ^2 (or, more precisely, $\ell^2(\mathbb{Z})$) of square-summable sequences of real or complex numbers.[1] That is, ℓ^2 consists of all infinite sequences $\{\ldots, c_{-2}, c_{-1}, c_0, c_1, c_2, \ldots\}$, $c_k \in \mathbb{K}$, for which

$$\sum_{k=-\infty}^{\infty} |c_k|^2 < \infty.$$

Another example of a Hilbert space one might have seen is the space $L^2(\mathbb{R})$ of square-integrable complex-valued functions on $\mathbb{R}$, that is, of all functions[2] $f : \mathbb{R} \to \mathbb{K}$ for which

$$\int_{-\infty}^{\infty} dx\, |f(x)|^2 < \infty.$$

In view of their special nature, it may therefore come as a surprise that Hilbert spaces play a central role in many areas of mathematics, notably in analysis, but also including (differential) geometry, group theory, stochastics, and even number theory. In addition, the notion of a Hilbert space provides the mathematical foundation of quantum mechanics. Indeed, the definition of a Hilbert space was first given by von Neumann (rather than Hilbert!) in 1927 precisely for the latter purpose. However, despite his exceptional brilliance, even von Neumann would probably not have been able to do so without the preparatory work in pure mathematics by Hilbert and others, which produced numerous constructions (like the ones mentioned above) that are now regarded as examples of the abstract notion of a Hilbert space. It is quite remarkable how a particular development within pure mathematics crossed one in theoretical physics in this way; this crossing is reminiscent to the one leading to the calculus around 1670; see below. Today, the most spectacular new application of Hilbert space theory is given by Noncommutative Geometry [3], where the motivation from pure mathematics is merged with the physical input from quantum mechanics. Consequently, this is an important field of research in pure mathematics as well as in mathematical physics.

In what follows, we shall separately trace the origins of the concept of a Hilbert space in mathematics and physics. As we shall see, Hilbert space theory is part of functional analysis, an area of mathematics that emerged between approximately 1880–1930. Functional analysis is almost indistinguishable from what is sometimes called 'abstract analysis' or 'modern analysis,'

[1] In what follows, we mainly work over the reals in order to serve intuition, but many infinite-dimensional vector spaces, especially Hilbert spaces, are defined over the complex numbers. Hence we will write our formulae in a way that is correct also for $\mathbb{C}$ instead of $\mathbb{R}$. Of course, for $z \in \mathbb{R}$ the expression $|z|^2$ is just z^2. We will occasionally use the fancy letter $\mathbb{K}$, for *Körper*, which in these notes stands for either $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$.

[2] As we shall see, the elements of $L^2(\mathbb{R})$ are, strictly speaking, not simply functions but equivalence classes of Borel functions. For detailed information we recommend the course *Maat en Integraal* by Professor A. van Rooij, which runs parallel to the present one.

which marked a break with classical analysis. The latter involves, roughly speaking, the study of properties of a single function, whereas the former deals with spaces of functions.[3] One may argue that classical analysis is tied to classical physics,[4] whereas modern analysis is associated with quantum theory. Of course, both kinds of analysis were largely driven by intrinsic mathematical arguments as well.[5] The final establishment of functional analysis and Hilbert space theory around 1930 was made possible by *combining* a concern for rigorous foundations with an interest in physical applications [2].

I.2 Origins in mathematics

Cf. [2, 4, 17, 22] for more information on the history of functional analysis and Hilbert spaces. The key idea behind functional analysis is to look at functions as points in some infinite-dimensional vector space. To appreciate the depth of this idea, it should be mentioned that the concept of a finite-dimensional vector space, today routinely taught to first-year students, only emerged in the work of Grassmann between 1844 and 1862 (to be picked up very slowly by other mathematicians because of the obscurity of Grassmann's writings), and that even the far less precise notion of a 'space' (other than a subset of $\mathbb{R}^n$) was not really known before the work of Riemann around 1850. Indeed, Riemann not only conceived the idea of a manifold (albeit in embryonic form, to be made rigorous only in the 20th century), whose points have a status comparable to points in $\mathbb{R}^n$, but also explicitly talked about spaces of functions (initially analytic ones, later also more general ones). However, Riemann's spaces of functions were not equipped with the structure of a vector space. In 1885 Weierstrass considered the distance between two functions (in the context of the calculus of variations), and in 1897 Hadamard took the crucial step of connecting the set-theoretic ideas of Cantor with the notion of a space of functions. Finally, in his PhD thesis of 1906, which is often seen as a turning point in the development of functional analysis, Hadamard's student Fréchet defined what is now called a metric space (i.e., a possibly infinite-dimensional vector space equipped with a metric, see below), and gave examples of such spaces whose points are functions.[6] After 1914, the notion of a topological space due to Hausdorff led to further progress, eventually leading to the concept of a topological vector space, which contains all spaces mentioned below as special cases.

To understand the idea of a space of functions, we first reconsider $\mathbb{R}^n$ as the space of all functions $f : \{1, 2, \ldots, n\} \to \mathbb{R}$, under the identification $x^1 = f(1), \ldots, x^n = f(n)$. Clearly, under this identification the vector space operations in $\mathbb{R}^n$ just correspond to pointwise operations on functions (e.g., $f + g$ is the function defined by $(f + g)(k) := f(k) + g(k)$, etc.). Hence $\mathbb{R}^n$ is a function space itself, consisting of functions defined on a finite set.

The given structure of $\mathbb{R}^n$ as a vector space may be enriched by defining the length $\|f\|$ of a vector f and the associated distance $d(f, g) = \|f - g\|$ between two vectors f and g. In addition,

[3] The modern concept of a function as a map $f : [a, b] \to \mathbb{R}$ was only arrived at by Dirichlet as late as 1837, following earlier work by notably Euler and Cauchy. But Newton already had an intuitive graps of this concept, at least for one variable.

[4] Classical analysis grew out of the calculus of Newton, which in turn had its roots in both geometry and physics. (Some parts of the calculus were later rediscovered by Leibniz.) In the 17th century, geometry was a practical matter involving the calculation of lenths, areas, and volumes. This was generalized by Newton into the calculus of integrals. Physics, or more precisely mechanics, on the other hand, had to do with velocities and accellerations and the like. This was abstracted by Newton into differential calculus. These two steps formed one of the most brilliant generalizations in the history of mathematics, crowned by Newton's insight that the operations of integration and differentiation are inverse to each other, so that one may speak of a unified differential and integral calculus, or briefly calculus. Attempts to extend the calculus to more than one variable and to make the ensuing machinery mathematically rigorous in the modern sense of the word led to classical analysis as we know it today. (Newton used theorems and proofs as well, but his arguments would be called "heuristic" or "intuitive" in modern mathematics.)

[5] The jump from classical to modern analysis was as discontinuous as the one from classical to quantum mechanics. The following anecdote may serve to illustrate this. G.H. Hardy was one of the masters of classical analysis and one of the most famous mathematicians altogether at the beginning of the 20th century. John von Neumann, one of the founders of modern analysis, once gave a talk on this subject at Cambridge in Hardy's presence. Hardy's comment was: "*Obviously a very intelligent man. But was that mathematics?*"

[6] Fréchet's main example was $C[a, b]$, seen as a metric space in the supremum-norm, i.e., $d(f, g) = \|f - g\|$ with $\|f\| = \sup\{f(x) \mid x \in [a, b]\}$.

the angle θ between f and g in $\mathbb{R}^n$ is defined. Lengths and angles can both be expressed through the usual inner product

$$(f,g) = \sum_{k=1}^{n} \overline{f(k)} g(k) \tag{I.1}$$

through the relations

$$\|f\| = \sqrt{(f,f)} \tag{I.2}$$

and

$$(f,g) = \|f\|\|g\| \cos\theta. \tag{I.3}$$

In particular, one has a notion of orthogonality of vectors, stating that f and g are orthogonal whenever $(f,g) = 0$, and an associated notion of orthogonality of subspaces:[7] we say that $V \subset \mathbb{R}^n$ and $W \subset \mathbb{R}^n$ are orthogonal if $(f,g) = 0$ for all $f \in V$ and $g \in W$. This, in turn, enables one to define the (orthogonal) projection of a vector on a subspace of $\mathbb{R}^n$.[8] Even the dimension n of $\mathbb{R}^n$ may be recovered from the inner product as the cardinality of an arbitrary orthogonal basis.[9]

Now replace $\{1, 2, \ldots, n\}$ by an infinite set. In this case the corresponding space of functions will obviously be infinite-dimensional in a suitable sense.[10] The simplest example is $\mathbb{N} = \{1, 2, \ldots, \}$, so that one may define $\mathbb{R}^\infty$ as the space of all functions $f : \mathbb{N} \to \mathbb{R}$, with the associated vector space structure given by pointwise operations. However, although $\mathbb{R}^\infty$ is well defined as a vector space, it turns out to be impossible to define an inner product on it, or even a length or distance. Indeed, defining

$$(f,g) = \sum_{k=1}^{\infty} \overline{f(k)} g(k) \tag{I.4}$$

it is clear that the associated length $\|f\|$ (still given by (I.2)) is infinite for most f. This is hardly surprising, since there are no growth conditions on f at infinity. The solution is to simply restrict $\mathbb{R}^\infty$ to those functions with $\|f\| < \infty$. These functions by definition form the set $\ell^2(\mathbb{N})$, which is easily seen to be a vector space. Moreover, it follows from the Cauchy–Schwarz inequality

$$(f,g) \leq \|f\|\|g\| \tag{I.5}$$

that the inner product is finite on $\ell^2(\mathbb{N})$. Consequently, the entire geometric structure of $\mathbb{R}^n$ in so far as it relies on the notions of lengths and angles (including orthogonality and orthogonal projections) is available on $\ell^2(\mathbb{N})$. Running ahead of the precise definition, we say that $\mathbb{R}^n \cong \ell^2(\{1, 2, \ldots, n\})$ is a finite-dimensional Hilbert space, whereas $\ell^2(\mathbb{N})$ is an infinite-dimensional one. Similarly, one may define $\ell^2(\mathbb{Z})$ (or indeed $\ell^2(S)$ for any countable set S) as a Hilbert space in the obvious way.

From a modern perspective, $\ell^2(\mathbb{N})$ or $\ell^2(\mathbb{Z})$ are the simplest examples of infinite-dimensional Hilbert spaces, but historically these were not the first to be found.[11] The initial motivation for the concept of a Hilbert space came from the analysis of integral equations[12] of the type

$$f(x) + \int_a^b dy\, K(x,y) f(y) = g(x), \tag{I.6}$$

[7] A subspace of a vector space is by definition a linear subspace.

[8] This is most easily done by picking a basis $\{e_i\}$ of the particular subspace V. The projection pf of f onto V is then given by $pf = \sum_i (e_i, f) e_i$.

[9] This is the same as the cardinality of an arbitrary basis, as any basis can be replaced by an orthogonal one by the Gram–Schmidt procedure.

[10] The dimension of a vector space is defined as the cardinality of some basis. The notion of a basis is complicated in general, because one has to distinguish between algebraic (or Hamel) and topological bases. Either way, the dimension of the spaces described below is infinite, though the cardinality of the infinity in question depends on the type of basis. The notion of an algebraic basis is very rarely used in the context of Hilbert spaces (and more generally Banach spaces), since the ensuing dimension is either finite or uncountable. The dimension of the spaces below with respect to a topological basis is countably infinite, and for a Hilbert space all possible cardinalities may occur as a possible dimension. In that case one may restrict oneself to an orthogonal basis.

[11] From the point of view of most mathematicians around 1900, a space like $\ell^2(\mathbb{N})$ would have been far to abstract to merit consideration.

[12] Integral equations were initially seen as reformulations of differential equations. For example, the differential equation $Df = g$ or $f'(x) = g(x)$ for unknown f is solved by $f = \int g$ or $f(x) = \int_0^x dy\, g(y) = \int_0^1 dy\, K(x,y) g(y)$ for $K(x,y) = \theta(x-y)$ (where $x \leq 1$), which is an integral equation for g.

where f, g, and K are continuous functions and f is unknown. Such equations were first studied from a somewhat modern perspective by Volterra and Fredholm around 1900, but the main breakthrough came from the work of Hilbert between 1904–1910. In particular, Hilbert succeeded in relating integral equations to an infinite-dimensional generalization of linear algebra by choosing an orthonormal basis $\{e_k\}$ of continuous functions on $[a,b]$ (such as $e_k(x) := \exp(2\pi kix)$ on the interval $[0,1]$), and defining the (generalized) Fourier coefficents of f by $\hat{f}_k := (e_k, f)$ with respect to the inner product

$$(f,g) := \int_a^b dx\, \overline{f(x)} g(x). \tag{I.7}$$

The integral equation (I.6) is then transformed into an equation of the type

$$\hat{f}_k = \sum_l \hat{K}_{kl} \hat{f}_l = \hat{g}_l. \tag{I.8}$$

Hilbert then noted from the Parseval relation (already well known at the time from Fourier analysis and more general expansions in eigenfunctions)

$$\sum_{k\in\mathbb{Z}} |\hat{f}_k|^2 = \int_a^b dx\, |f(x)|^2 \tag{I.9}$$

that the left-hand side is finite, so that $\hat{f} \in \ell^2(\mathbb{Z})$. This, then, led him and his students to study ℓ^2 also abstractly. E. Schmidt should be mentioned here in particular. Unlike Hilbert, already in 1908 he looked at ℓ^2 as a 'space' in the modern sense, thinking of seqences (c_k) as point in this space. Schmidt studied the geometry of ℓ^2 as a Hilbert space in the modern sense, that is, empasizing the inner product, orthogonality, and projections, and decisively contributed to Hilbert's work on spectral theory.

The space $L^2(a,b)$ appeared in 1907 in the work of F. Riesz[13] and Fischer as the space of (Lebesgue) integrable functions[14] on (a,b) for which

$$\int_a^b dx\, |f(x)|^2 < \infty;$$

of course, this condition holds if f is continuous on $[a,b]$. Equipped with the inner product (I.7), this was another early example of what is now called a Hilbert space.[15] The context of its appearance was what is now called the Riesz–Fischer theorem: *Given any sequence (c_k) of real (or complex) numbers and any orthonormal system (e_k) in $L^2(a,b)$,*[16] *there exists a function $f \in L^2(a,b)$ for which $(e_k, f) = c_k$ if and only if $c \in \ell^2$, i.e., if $\sum_k |c_k|^2 < \infty$.*

At the time, the Riesz–Fischer theorem was completely unexpected, as it proved that two seemingly totally different spaces were 'the same' from the right point of view. In modern terminology, the theorem establishes an isomorphism of ℓ^2 and L^2 as Hilbert spaces, but this point of view was only established twenty years later, i.e., in 1927, by von Neumann. Inspired by quantum mechanics (see below), in that year von Neumann gave the definition of a Hilbert space as an abstract mathematical structure, as follows. First, an **inner product** on a vector space V over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$), is a map $V \times V \to \mathbb{K}$, written as $\langle f, g\rangle \mapsto (f,g)$, satisfying, for all $f, g \in V$ and $t \in \mathbb{K}$,

1. $(f,f) \geq 0$;
2. $(g,f) = \overline{(f,g)}$;

[13] Frederic Riesz had a brother, Marcel Riesz, who was a well-known mathematician too.

[14] More precisely, the elements of $L^2(a,b)$ are not functions but equivalence classes thereof, where $f \sim g$ when $\|f-g\|_2 = 0$.

[15] The term 'Hilbert space' was first used by Schoenflies in 1908 for ℓ^2, and was introduced in the abstract sense by von Neumann in 1927; see below.

[16] The notion of an orthonormal system of functions on the interval $[a,b]$ was as old as Fourier, and was defined abstractly by Hilbert in 1906.

3. $(f, tg) = t(f, g)$;
4. $(f, g + h) = (f, g) + (f, h)$;
5. $(f, f) = 0 \Rightarrow f = 0$.

Given an inner product on V, one defines an associated length function or norm (see below) $\|\cdot\| : V \to \mathbb{R}^+$ by (I.2). A **Hilbert space** (over $\mathbb{K}$) is a vector space (over $\mathbb{K}$) with inner product, with the property that Cauchy sequences with respect to the given norm are convergent (in other words, V is complete in the given norm).[17] Hilbert spaces are denoted by the letter H rather than V. Thus Hilbert spaces preserve as much as possible of the geometry of $\mathbb{R}^n$.

It can be shown that the spaces mentioned above are Hilbert spaces. Defining an **isomorphism** of Hilbert spaces $U : H_1 \to H_2$ as an invertible linear map preserving the inner product (i.e., $(Uf, Ug)_2 = (f, g)_1$ for all $f, g \in H_1$), the Riesz–Fischer theorem shows that $\ell^2(\mathbb{Z})$ and $L^2(a, b)$ are indeed isomorphic.

In a Hilbert space the inner product is fundamental, the norm being derived from it. However, one may instead take the norm as a starting point (or, even more generally, the metric, as done by Fréchet in 1906). The abstract properties of a norm were first identified by Riesz in 1918 as being satisfied by the supremum norm, and were axiomatized by Banach in his thesis in 1922. A **norm** on a vector space V over a field $\mathbb{K}$ as above is a function $\|\cdot\| : V \to \mathbb{R}^+$ with the properties:

1. $\|f + g\| \leq \|f\| + \|g\|$ for all $f, g \in V$;
2. $\|tf\| = |t|\|f\|$; for all $f \in V$ and $t \in \mathbb{K}$;
3. $\|f\| = 0 \Rightarrow f = 0$.

The usual norm on $\mathbb{R}^n$ satisfies these axioms, but there are many other possibilities, such as

$$\|f\|_p := \left(\sum_{k=1}^{n} |f(k)|^p \right)^{1/p} \tag{I.10}$$

for any $p \in \mathbb{R}$ with $1 \leq p < \infty$, or

$$\|f\|_\infty := \sup\{|f(k)|, k = 1, \ldots, n\}.$$

In the finite-dimensional case, these norms (and indeed all other norms) are all equivalent in the sense that they lead to the same criterion of convergence (technically, they generate the same topology): if we say that $f_n \to f$ when $\|f_n - f\| \to 0$ for some norm on $\mathbb{R}^n$, then this implies convergence with respect to any other norm. This is no longer the case in infinite dimension. For example, one may define $\ell^p(\mathbb{N})$ as the subspace of $\mathbb{R}^\infty$ that consists of all vectors $f \in \mathbb{R}^\infty$ for which

$$\|f\|_p := \left(\sum_{k=1}^{\infty} |f(k)|^p \right)^{1/p} \tag{I.11}$$

is finite. It can be shown that $\|\cdot\|_p$ is indeed a norm on $\ell^p(\mathbb{N})$, and that this space is complete in this norm. As with Hilbert spaces, the examples that originally motivated Riesz to give his definition were not ℓ^p spaces but the far more general L^p spaces, which he began to study in 1910. For example, $L^p(a, b)$ consists of all (equivalence classes of Lebesgue) integrable functions f on (a, b) for which

$$\|f\|_p := \left(\int_a^b dx\, |f(x)|^p \right)^{1/p} \tag{I.12}$$

[17] A sequence (f_n) is a Cauchy sequence in V when $\|f_n - f_m\| \to 0$ when $n, m \to \infty$; more precisely, for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $\|f_n - f_m\| < \varepsilon$ for all $n, m > N$. A sequence (f_n) converges if there is $f \in V$ such that $\lim_{n\to\infty} \|f_n - f\| = 0$.

is finite, still for $1 \leq p < \infty$, and also $\|f\|_\infty := \sup\{|f(x)|, x \in (a,b)\}$. Eventually, in 1922 Banach defined what is now called a **Banach space** as a vector space (over $\mathbb{K}$ as before) that is complete in some given norm.

Long before the abstract definitions of a Hilbert space and a Banach space were given, people began to study the infinite-dimensional generalization of functions on $\mathbb{R}^n$. In the hands of Volterra, the calculus of variations originally inspired the study of functions $\varphi : V \to \mathbb{K}$, later called **functionals**, and led to early ideas about possible continuity of such functions. However, although the calculus of variations involved nonlinear functionals as well, only linear functionals turned out to be tractable at the time (until the emergence of nonlinear functional analysis much later). Indeed, even today (continuous) linear functionals still form the main scalar-valued functions that are studied on infinite-dimensional (topological) vector spaces. For this reason, throughout this text a **functional** will denote a **continuous linear functional**. For $H = L^2(a,b)$, it was independently proved by Riesz and Fréchet in 1907 that any functional on H is of the form $g \mapsto (f,g)$ for some $f \in H$.[18] The same result for arbitrary Hilbert spaces H was written down only in 1934–35, again by Riesz, although it is not very difficult.

The second class of 'functions' on Hilbert spaces and Banach spaces that could be analyzed in detail were the generalizations of matrices on $\mathbb{R}^n$, that is, linear maps from the given space to itself. Such functions are now called operators.[19] For example, the integral equation (I.6) is then simply of the form $(1+K)f = g$, where $1 : L^2(a,b) \to L^2(a,b)$ is the identity operator $1f = f$, and $K : L^2(a,b) \to L^2(a,b)$ is the operator given by $(Kf)(x) = \int_a^b dy\, K(x,y)f(y)$. This is easy for us to write down, but in fact it took some time before integral of differential equations were interpreted in terms of operators acting on functions.[20] They managed to generalize practically all results of linear algebra to operators, notably the existence of a complete set of eigenvectors for operators of the stated type with symmetric kernel, that is, $K(x,y) = K(y,x)$.[21]

The abstract concept of a (bounded) operator (between what we now call Banach spaces) is due to Riesz in 1913. It turned out that Hilbert and Schmidt had studied a special class of operators we now call 'compact', whereas an even more famous student of Hilbert's, Weyl, had investigated a singular class of operators now called 'unbounded' in the context of ordinary differential equations. Spectral theory and eigenfunctions expansions were studied by Riesz himself for general bounded operators on Hilbert spaces (seen by him as a special case of general normed spaces), and later, more specifically in the Hilbert space case, by Hellinger and Toeplitz (culminating in their pre-von Neumann review article of 1927).

In the Hilbert space case, the results of all these authors were generalized almost beyond recognition by von Neumann in his book from 1932 [15], to whose origins we now turn.

I.3 Origins in physics

For more details on the origin of the Hilbert space concept in physics see [9, 11, 14]. For biographical information on John von Neumann[22] see [6, 7, 13, 25].

From 1900 onwards, physicists had begun to recognize that the classical physics of Newton, Maxwell and Lorentz (i.e., classical mechanics, Newtonian gravity, and electrodynamics) could not describe all of Nature. The fascinating era that was thus initiated by Planck, to be continued

[18] More generally, in 1910 Riesz showed that any functional on $L^p(a,b)$ is given by an element $L^q(a,b)$, where $1/p + 1/q = 1$, by the same formula. Since $p = 2$ implies $q = 2$, this of course implies the earlier Hilbert space result.

[19] Or *linear* operators, but for us linearity is part of the definition of an operator.

[20] For example, Hilbert and Schmidt did not really have the operator concept but (from the modern point of view) worked in terms of the associated quadratic form. That is, the operator $a : H \to H$ defines a map $q : H \times H \to \mathbb{K}$ by $\langle f,g\rangle \mapsto (f,ag)$.

[21] The associated quadratic form then satisfies $\overline{q(f,g)} = q(g,f)$.

[22] John von Neumann (1903–1957) was a Hungarian prodigy; he wrote his first mathematical paper at the age of seventeen. Except for this first paper, his early work was in set theory and the foundations of mathematics. In the Fall of 1926, he moved to Göttingen to work with Hilbert, the most prominent mathematician of his time. Around 1920, Hilbert had initiated his *Beweistheory*, an approach to the axiomatization of mathematics that was doomed to fail in view of Gödel's later work. However, at the time that von Neumann arrived, Hilbert was mainly interested in quantum mechanics; see below.

mainly by Einstein, Bohr, and De Broglie, ended in 1925–1927 with the discovery of quantum mechanics. This theory replaced classical mechanics, and was initially discovered in two guises.

First, Heisenberg discovered a form of quantum mechanics that at the time was called 'matrix mechanics.' Heisenberg's basic idea was that in atomic physics physical observables (that is, measurable quantities) should not depend on continuous variables like position and momentum (as he did not believe the concept of an electronic orbit in an atom made sense), but on discrete quantities, like the natural numbers $n = 1, 2, 3, \ldots$ labelling the orbits in Bohr's model of the atom. Specifically, Heisenberg thought that in analogy to a 'quantum jump' from one orbit to the other, everything should be expressed in terms of two such numbers. Thus he replaced the functions $f(x, p)$ of position and momentum in terms of which classical physics is formulated by quantities $f(m, n)$. In order to secure the law of conservation of energy in his new mechanics, he was forced to postulate the multiplication rule $f * g(m, n) = \sum_l f(m, l)g(l, n)$, replacing the rule $fg(x, p) = f(x, p)g(x, p)$ of classical mechanics. He noted that $f * g \neq g * f$, unlike in classical mechanics, and saw in this non-commutativity of physical observables the key revolutionary character of quantum mechanics. When he showed his work to his boss Born, a physicist who as a former assistant to Hilbert was well versed in mathematics, Born saw, after a sleepless night, that Heisenberg's multiplication rule was the same as the one known for matrices, but now of infinite size.[23] Thus Heisenberg's embryonic formulation of quantum theory, written down in 1925 in a paper generally seen as the birth of quantum mechanics, came to be known as 'matrix mechanics'.

Second, Schrödinger was led to a formulation of quantum theory called 'wave mechanics', in which the famous symbol Ψ, denoting a 'wave function,' played an important role. To summarize a long story, Schrödinger based his work on de Broglie's idea that in quantum theory a wave should be associated to each particle; this turned Einsteins's concept of a photon from 1905 on its head.[24] De Broglie's waves should, of course, satisfy some equation, similar to the fundamental wave equation or Maxwell's equations. It is this equation that Schrödinger proposed in 1926 and which is now named after him.[25] Schrödinger found his equation by studying the transition from wave optics to geometric optics, and by (wrongly) believing that there should be a similar transition from wave mechanics to classical mechanics.[26]

Thus in 1926 one had two alternative formulations of quantum mechanics, which looked completely different, but each of which could explain certain atomic phenomena. The relationship and possible equivalence between these formulations was, of course, much discussed at the time. The most obvious difficulty in relating Heisenberg's work to Schrödinger's was that the former was a theory of observables lacking the concept of a state, whereas the latter had precisely the opposite feature: Schrödinger's wave functions were states, but where were the observables? To answer this question, Schrödinger introduced his famous expressions $Q = x$ (more precisely, $Q\Psi(x) = x\Psi(x)$) and $P = -i\hbar\partial/\partial x$, defining what we now call unbounded operators on the Hilbert space $L^2(\mathbb{R}^3)$. Subsequently, Dirac, Pauli, and Schrödinger himself recognized that wave mechanics was related to matrix mechanics in the following way: Heisenberg's matrix $x(m, n)$ was nothing but the matrix element (e_n, Qe_m) of the position operator Q with respect to the orthonormal basis of $L^2(\mathbb{R}^3)$ given by the eigenfunctions of the Hamiltonian $H = P^2/2m + V(Q)$. Conversely, the vectors in ℓ^2 on which Heisenberg's matrices acted could be interpreted as states. However, these observations fell far short of an equivalence proof of wave mechanics and matrix mechanics (as is sometimes claimed), let alone of a mathematical understanding of quantum mechanics.

Heisenberg's paper was followed by the 'Dreimännerarbeit' of Born, Heisenberg, and Jordan

[23] At the time, matrices and linear algebra were unknown to practically all physicists.

[24] Einstein's revolutionary proposal, which marked the true conceptual beginning of quantum theory, had been that light, universally seen as a wave phenomenon at the time, had a particle nature as well. The idea that light consists of particles had earlier been proposed by none other than Newton, but had been discredited after the discovery of Young around 1800 (and its further elaboration by Fresnel) that light displayes interference phenomena and therefore should have a wave nature. This was subsequently confirmed by Maxwell's theory, in which light is an oscillation of the electromagnetic field. In his PhD thesis from 1924, de Broglie generalized and inverted Einstein's reasoning: where the latter had proposed that light waves are particles, the former postulated that particles are waves.

[25] He first found the time-independent Schrödinger equation $H\Psi = E\Psi$ with $H = -\hbar^2\Delta/2m+V$, and subsequently got the time-dependent one $H\Psi = i\hbar\partial\Psi/\partial t$.

[26] Technically, Schrödinger relied on the Hamilton–Jacobi formulation of classical mechanics.

(1926); all three were in Göttingen at the time. Born turned to his former teacher Hilbert for mathematical advice. Hilbert had been interested in the mathematical structure of physical theories for a long time; his Sixth Problem (1900) called for the mathematical axiomatization of physics. Aided by his assistants Nordheim and von Neumann, Hilbert ran a seminar on the mathematical structure of quantum mechanics, and the three wrote a joint paper on the subject (now obsolete).

It was von Neumann alone who, at the age of 23, recognized the mathematical structure of quantum mechanics. In this process, he defined the abstract concept of a Hilbert space discussed above; as we have said, previously only some examples of Hilbert spaces had been known. Von Neumann saw that Schrödinger's wave functions were unit vectors in the Hilbert space $L^2(\mathbb{R}^3)$, and that Heisenberg's observables were linear operators on the Hilbert space ℓ^2. The Riesz–Fischer theorem then implied the mathematical equivalence between wave mechanics and matrix mechanics. In a series of papers that appeared between 1927–1929, von Neumann defined Hilbert space, formulated quantum mechanics in this language, and developed the spectral theory of bounded as well as unbounded normal operators on a Hilbert space. This work culminated in his book [15], which to this day remains the definitive account of the mathematical structure of elementary quantum mechanics.[27]

Von Neumann proposed the following mathematical formulation of quantum mechanics. The observables of a given physical system are the self-adjoint (possibly unbounded) linear operators a on a Hilbert space H. The pure states of the system are the unit vectors in H. The expectation value of an observable a in a state ψ is given by $(\psi, a\psi)$. The transition probability between two states ψ and φ is $|(\psi, \varphi)|^2$. As we see from (I.3), this number is just $(\cos\theta)^2$, where θ is the angle between the unit vectors ψ and φ. Thus the geometry of Hilbert space has a direct physical interpretation in quantum mechanics, surely one of von Neumann's most brilliant insights. Later on, he would go beyond his Hilbert space approach to quantum theory by developing such topics and quantum logic (see [1]) and operator algebras (cf. [3]).

[27] Von Neumann's book was preceded by Dirac's *The Principles of Quantum Mechanics* (1930), which contains another brilliant, but this time mathematically questionable account of quantum mechanics in terms of linear spaces and operators.

Chapter II

Metric spaces, normed spaces, and Hilbert spaces

II.1 Basic definitions

We repeat two basic definitions from the Introduction, and add a third:

Definition II.1 *Let V be a vector space over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$).*

An **inner product** *on V is a map $V \times V \to \mathbb{K}$, written as $\langle f, g\rangle \mapsto (f, g)$, satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $(f, f) \in \mathbb{R}^+ := [0, \infty)$ *(positivity);*
2. $(g, f) = \overline{(f, g)}$ *(symmetry);*
3. $(f, tg) = t(f, g)$ *(linearity 1);*
4. $(f, g + h) = (f, g) + (f, h)$ *(linearity 2);*
5. $(f, f) = 0 \Rightarrow f = 0$ *(positive definiteness).*

A **norm** *on V is a function $\|\cdot\| : V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $\|f + g\| \leq \|f\| + \|g\|$ *(triangle inequality);*
2. $\|tf\| = |t|\|f\|$ *(homogeneity);*
3. $\|f\| = 0 \Rightarrow f = 0$ *(positive definiteness).*

A **metric** *on V is a function $d : V \times V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$:*

1. $d(f, g) \leq d(f, h) + d(h, g)$ *(triangle inequality);*
2. $d(f, g) = d(g, f)$ *for all $f, g \in V$ (symmetry);*
3. $d(f, g) = 0 \Leftrightarrow f = g$ *(definiteness).*

The notion of a metric applies to any set, not necessarily to a vector space, like an inner product and a norm. These structures are related in the following way:[1]

[1] Apart from a norm, an inner product defines another structure called a **transition probability**, which is of great importance to quantum mechanics; cf. the Introduction. Abstractly, a transition probability on a set S is a function $p : S \times S \to [0, 1]$ satisfying $p(x, y) = 1 \Leftrightarrow x = y$ (cf. Property 3 of a metric) and $p(x, y) = p(y, x)$. See [10]. Now take the set S of all vectors in a complex inner product space that have norm 1, and define an equivalence relation on S by $f \sim g$ iff $f = zg$ for some $z \in \mathbb{C}$ with $|z| = 1$. (Without taking equivalence classes the first axiom would not be satisfied). The set $S = \mathsf{S}/\sim$ is then equipped with a transition probability defined by $p([f], [g]) := |(f, g)|^2$. Here $[f]$ is the equivalence class of f with $\|f\| = 1$, etc. In quantum mechanics vectors of norm 1 are (pure) states, so that the transition probability between two states is determined by their angle θ. (Recall the elementary formula from Euclidean geometry $(x, y) = \|x\|\|y\| \cos\theta$, where θ is the angle between x and y in $\mathbb{R}^n$.)

Proposition II.2 *1. An inner product on V defines a norm on V by means of $\|f\| = \sqrt{(f,f)}$.*

2. A norm on V defines a metric on V through $d(f,g) := \|f-g\|$.

The proof of this claim is an easy exercise; part 1 is based on the **Cauchy–Schwarz inequality**

$$|(f,g)| \leq \|f\|\|g\|, \tag{II.1}$$

whose proof in itself is an exercise, and part 2 is really trivial: the three axioms on a norm immediately imply the corresponding properties of the metric. The question arises when a norm comes from an inner product in the stated way: this question is answered by the **Jordan–von Neumann theorem**:

Theorem II.3 *A norm $\|\cdot\|$ on a vector space comes from an inner product through $\|f\| = \sqrt{(f,f)}$ if and only if*

$$\|f+g\|^2 + \|f-g\|^2 = 2(\|f\|^2 + \|g\|^2). \tag{II.2}$$

In that case, one has

$$4(f,g) = \|f+g\|^2 - \|f-g\|^2 \quad \text{for } \mathbb{K} = \mathbb{R}$$

and

$$4(f,g) = \|f+g\|^2 - \|f-g\|^2 + i\|f-ig\|^2 - i\|f+ig\|^2 \quad \text{for } \mathbb{K} = \mathbb{C}.$$

We leave the proof of this theorem as an exercise as well, though it is by no means trivial.

Applied to the ℓ^p and L^p spaces mentioned in the introduction, this yields the result that the norm in these spaces comes from an inner product if and only if $p = 2$; see below for a precise definition of $L^p(\Omega)$ for $\Omega \subseteq \mathbb{R}^n$. There is no (known) counterpart of this result for the transition from a norm to a metric.[2] It is very easy to find examples of metrics that do not come from a norm: on any vector space (or indeed any set) V the formula $d(f,g) = \delta_{fg}$ defines a metric not derived from a norm. Also, if d is any metric on V, then $d' = d/(1+d)$ is a metric, too: since cleary $d'(f,g) \leq 1$ for all f, g, this metric can never come from a norm.

II.2 Convergence and completeness

The reason we look at metrics in a Hilbert space course is, apart from general education, that many concepts of importance for Hilbert spaces are associated with the metric rather than with the underlying inner product or norm. The main such concept is convergence:

Definition II.4 *Let $(x_n) := \{x_n\}_{n\in\mathbb{N}}$ be a sequence in a metric space (V,d). We say that $x_n \to x$ (i.e., (x_n) converges to $x \in V$) when $\lim_{n\to\infty} d(x_n, x) = 0$, or, more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon$ for all $n > N$.*

In a normed space, hence in particular in a space with inner product, this therefore means that $\lim_{n\to\infty} \|x_n - x\| = 0$.[3]

A sequence (x_n) in (V,d) is called a **Cauchy sequence** when $d(x_n, x_m) \to 0$ when $n, m \to \infty$; more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x_m) < \varepsilon$ for all $n, m > N$. Clearly, a convergent sequence is Cauchy: from the triangle inequality and symmetry one has

$$d(x_n, x_m) \leq d(x_n, x) + d(x_m, x).$$

So for given $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon/2$, etcetera. However, the converse statement does not hold in general, as is clear from the example of the metric space $(0,1)$ with metric $d(x,y) = |x-y|$: the sequence $x_n = 1/n$ does not converge in $(0,1)$ (for an example involving a vector space see the exercises). In this case one can simply extend the given space to $[0,1]$, in which every Cauchy sequence does converge.

[2] More generally, a metric (on an arbitrary set) defines a so-called topology on this set, but we leave this to the Topology course by F. Clauwens.

[3] Such convergence is sometimes called **strong convergence**, in contrast to **weak convergence**, which for an inner product space means that $\lim_n |(y, x_n - x)| = 0$ for each $y \in V$.

Definition II.5 *A metric space (V, d) is called* **complete** *when every Cauchy sequence converges.*

- *A vector space with norm that is complete in the associated metric is called a* **Banach space**.
- *A vector space with inner product that is complete in the associated metric is called a* **Hilbert space**.

The last part may be summarized as follows: *a vector space H with inner product $(\ ,\ )$ is a Hilbert space when every sequence (x_n) such that $\lim_{n,m\to\infty} \|x_n - x_m\| = 0$ has a limit $x \in H$ in the sense that $\lim_{n\to\infty} \|x_n - x\| = 0$ (where $\|x\| = \sqrt{(x,x)}$).* It is easy to see that such a limit is unique.

Like any good definition, this one too comes with a theorem:

Theorem II.6 *For any metric space (V, d) there is a complete metric space $(\tilde{V}, \tilde{d})$ (unique up to isomorphism) containing (V, d) as a dense subspace*[4] *on which $\tilde{d} = d$. If V is a vector space, then so is $\tilde{V}$. If the metric d comes from a norm, then $\tilde{V}$ carries a norm inducing $\tilde{d}$ (so that $\tilde{V}$, being complete, is a Banach space). If the norm on V comes from an inner product, then $\tilde{V}$ carries an inner product, which induces the norm just mentioned (so that $\tilde{V}$ is a Hilbert space), and whose restriction to V is the given inner product.*

Since this theorem is well known and basic in analysis (see [28], §9.5.2., pp. 24–27), we will not give a complete proof, but will just sketch the main idea. In this course one only needs the case where the metric comes from a norm, so that $d(x_n, y_n) = \|x_n - y_n\|$ etc. in what follows.

One defines the completion $\tilde{V}$ as the set of all Cauchy sequences (x_n) in V, modulo the equivalence relation $(x_n) \sim (y_n)$ when $\lim_n d(x_n, y_n) = 0$. (When x_n and y_n converge in V, this means that they are equivalent when they have the same limit.) The metric $\tilde{d}$ on the set of such equivalence classes $[x_n] := [(x_n)]$ is defined by $\tilde{d}([x_n], [y_n]) := \lim_n d(x_n, y_n)$.[5] The embedding $\iota : V \hookrightarrow \tilde{V}$ is given by identifying $x \in V$ with the Cauchy sequence $(x_n = x\,\forall n)$, i.e., $\iota(x) = [x_n = x]$. It follows that a Cauchy sequence (x_n) in $V \subseteq \tilde{V}$ converges to $[x_n]$, for

$$\lim_m \tilde{d}(\iota(x_m), [x_n]) = \lim_m \tilde{d}([x_n = x_m], [x_n]) = \lim_m \lim_n d(x_m, x_n) = 0$$

by definition of a Cauchy sequence. Furthermore, one can show that any Cauchy sequence in $\tilde{V}$ converges by approximating its elements by elements of V.

If V is a vector space, the corresponding linear structure on $\tilde{V}$ is given by $[x_n]+[y_n] := [x_n+y_n]$ and $t[x_n] := [tx_n]$. If V has a norm, the corresponding norm on $\tilde{V}$ is given by $\|[x_n]\| := \lim_n \|x_n\|$.[6]

If V has an inner product, the corresponding inner product on $\tilde{V}$ is given by $([x_n], [y_n]) := \lim_n (x_n, y_n)$.[7] ■

A finite-dimensional vector space is complete in any possible norm. In infinite dimension, completeness generally depends on the norm (which often can be chosen in many different ways, even apart from trivial operations like rescaling by a positive constant). For example, take $V = \ell_c$, the space of functions $f : \mathbb{N} \to \mathbb{C}$ (or, equivalently, of infinite sequence $(f(1), f(2), \ldots, f(k), \ldots)$) with only finitely many $f(k) \neq 0$. Two interesting norms on this space are:

$$\|f\|_\infty := \sup_k \{|f(k)|\}; \tag{II.3}$$

$$\|f\|_2 := \left(\sum_{k=1}^{\infty} |f(k)|^2 \right)^{1/2}. \tag{II.4}$$

[4] This means that any point in $\tilde{V}$ is the limit of some convergent sequence in V with respect to the metric $\tilde{d}$.

[5] This limit exists, since using the triangle inequality one easily shows that $|d(x_n, y_n) - d(x_m, y_m)| \leq d(x_n, x_m) + d(y_n, y_m)$.

[6] Note that $(\|x_n\|)$ is a Cauchy sequence in $\mathbb{R}$ (from the inequality $\|x_n\| - \|x_m\| \leq \|x_n - x_m\|$, which you get from the triangle inequality for the norm).

[7] The existence of this limit is an easy exercise: we write $(x_n, y_n) - (x_m, y_m) = (x_n - x_m, y_n) + (x_m, y_n - y_m)$ hence, from Cauchy-Schwarz, $|(x_n, y_n) - (x_m, y_m)| \leq \|x_n - x_m\|\|y_n\| + \|y_n - y_m\|\|x_m\|$. Since $\|y_n\|$ and $\|x_m\|$ are Cauchy, hence convergent (see previous footnote), hence bounded, (x_n, y_n) is a Cauchy sequence in $\mathbb{C}$.

ℓ_c is not complete in either norm. However, the space

$$\ell^\infty := \{f : \mathbb{N} \to \mathbb{C} \mid \|f\|_\infty < \infty\} \tag{II.5}$$

is complete in the norm $\|\cdot\|_\infty$, and the space

$$\ell^2 := \{f : \mathbb{N} \to \mathbb{C} \mid \|f\|_2 < \infty\} \tag{II.6}$$

is complete in the norm $\|\cdot\|_2$. In fact, ℓ^2 is a Hilbert space in the inner product

$$(f, g) := \sum_{k=1}^{\infty} \overline{f(k)} g(k). \tag{II.7}$$

Now we seem to face a dilemma. One the one hand, there is the rather abstract completion procedure for metric spaces just sketched: it looks terrible to use in practice. On the other hand, we would like to regard ℓ^∞ as the completion of ℓ_c in the norm $\|\cdot\|_\infty$ and similarly we would like to see ℓ^2 as the completion of ℓ_c in the norm $\|\cdot\|_2$.

This can indeed be done through the following steps, which we just outline for the Hilbert space case ℓ^2 (similar comments hold for ℓ^∞ and are left to the reader):

1. Embed $V = \ell_c$ is some larger space W: in this case, W is the space of all sequences (or of all functions $f : \mathbb{N} \to \mathbb{C}$).
2. Guess a maximal subspace H of W in which the given norm $\|\cdot\|_2$ is finite: in this case this is $H = \ell^2$.
3. Prove that H is complete.
4. Prove that V is dense in H, in the sense that each element $f \in H$ is the limit of a Cauchy sequence in V.

The last step is usually quite easy. For example, any element $f \in \ell^2$ is the limit (with respect to the norm $\|\cdot\|_2$, of course), of the sequence (f_n) where $f_n(k) = f(k)$ if $k \leq n$ and $f_n(k) = 0$ if $k > n$. Clearly, $f_n \in \ell_c$ for all n.

The third step may in itself be split up in the following way:

- Take a generic Cauchy sequence (f_n) in H and guess its limit f in W.
- Prove that $f \in H$.
- Prove that $\lim_n \|f_n - f\| = 0$.

Here also the last step is often easy, given the previous ones.

In our example this procedure is implemented as follows.

- If (f_n) is any sequence in ℓ^2, the the definition of the norm implies that for each k one has

  $$|f_n(k) - f_m(k)| \leq \|f_n - f_m\|_2,$$

  So if (f_n) is a Cauchy sequence in ℓ^2, then for each k, $(f_n(k))$ is a Cauchy sequence in $\mathbb{C}$. Since $\mathbb{C}$ is complete, the latter has a limit called $f(k)$. This defines $f \in W$ as the candidate limit of (f_n), simply by $f : k \mapsto f(k) := \lim_n f_n(k)$.

- For each n one has:

  $$\|f_n - f\|_2^2 = \sum_{k=1}^{\infty} |f_n(k) - f(k)|^2 = \lim_{N\to\infty} \lim_{m\to\infty} \sum_{k=1}^{N} |f_n(k) - f_m(k)|^2.$$

  By the definition of lim sup and using the positivity of all terms one has

  $$\lim_{m\to\infty} \sum_{k=1}^{N} |f_n(k) - f_m(k)|^2 \leq \lim \sup_{m\to\infty} \sum_{k=1}^{\infty} |f_n(k) - f_m(k)|^2 = \lim \sup_{m\to\infty} \|f_n - f_m\|_2^2.$$

Hence

$$\|f_n - f\|_2^2 \leq \lim \sup_{m\to\infty} \|f_n - f_m\|_2^2.$$

Since (f_n) is Cauchy, this can be made $< \epsilon^2$ for $n > N$. Hence $\|f_n - f\|_2 \leq \epsilon$, so $f_n - f \in \ell^2$ and since $f_n \in \ell^2$ and ℓ^2 is a vector space, it follows that $f \in \ell^2 = H$, as desired.

- The claim $\lim_n \|f_n - f\| = 0$ follows from the same argument.

Returning to our dilemma, we wish to establish a link between the "practical" completion ℓ^2 of ℓ_c and the formal completion $\tilde{\ell_c}$. Such a link is given by the concept of **isomorphism** of two Hilbert spaces H_1 and H_2. As in the Introduction, we define an **isomorphism** of Hilbert spaces $U : H_1 \to H_2$ as an invertible linear map preserving the inner product (i.e., $(Uf, Ug)_2 = (f, g)_1$ for all $f, g \in H_1$). Such a map U is called a **unitary transformation** and we write $H_1 \cong H_2$.

So, in order to identify ℓ^2 with $\tilde{\ell_c}$ we have to find such a $U : \tilde{\ell_c} \to \ell^2$. This is easy: if (f_n) is Cauchy in ℓ_c we put

$$U([f_n]) := f = \lim_n f_n, \tag{II.8}$$

where f is the limit as defined above. It is an exercise to check that:

1. This map is well-defined, in the sense that if $f_n \sim g_n$ then $\lim_n f_n = \lim_n g_n$;
2. This map is indeed invertible and preserves the inner product.

We now apply the same strategy to a more complicated situation. Let $\Omega \subseteq \mathbb{R}^n$ be an open or closed subset of $\mathbb{R}^n$; just think of $\mathbb{R}^n$ itself for the quantum theory of a particle, of $[-\pi, \pi] \subset \mathbb{R}$ for Fourier analysis as done in Analysis 3 [28].[8] The role of ℓ_c in the previous analysis is now played by $C_c(\Omega)$, the vector space of complex-valued continuous functions on Ω with compact support.[9] Again, one has two natural norms on $C_c(\Omega)$:

$$\|f\|_\infty := \sup_{x\in\Omega}\{|f(x)|\}, \tag{II.9}$$

$$\|f\|_2 := \left(\int_\Omega d^n x\, |f(x)|^2\right)^{1/2}. \tag{II.10}$$

The first norm is called the **supremum-norm** or **sup-norm**. The second norm is called the **$\mathbf{L^2}$-norm** (see below). It is, of course, derived from the inner product

$$(f, g) := \int_\Omega d^n x\, \overline{f(x)} g(x). \tag{II.11}$$

But even the first norm will turn out to play an important role in Hilbert space theory.

Interestingly, if Ω is compact, then $C_c(\Omega) = C(\Omega)$ is complete in the norm $\|\cdot\|_\infty$. This claim follows from the theory of uniform convergence, which is not part of this course (see [28]).[10]

However, $C_c(\Omega)$ fails to be complete in the norm $\|\cdot\|_2$ (see exercises): Consider $\Omega = [0, 1]$. The sequence of functions

$$f_n(x) := \begin{cases} 0 & (x \leq 1/2) \\ n(x - 1/2) & (1/2 \leq x \leq 1/2 + 1/n) \\ 1 & (x \geq 1/2 + 1/n) \end{cases}$$

is a Cauchy sequence with respect to $\|\cdot\|_2$ that converges to a discontinuous function $f(x) = 0$ for $x \in [0, 1/2)$ and $f(x) = 1$ for $x \in (1/2, 1]$ (the value at $x = 1/2$ is not settled; see below, but in any case it cannot be chosen in such a way that f is continuous).

[8] More generally, Ω should be a so-called Borel subset of $\mathbb{R}^m$.

[9] The **support** of a function is defined as the smallest closed set outside which it vanishes.

[10] To cover the noncompact case, we introduce the space $C_0(\Omega)$ that consists of all continuous functions on Ω that vanish at infinity, in the sense that for each $\epsilon > 0$ there is a compact subset $K \subset \Omega$ such that $|f(x)| < \epsilon$ for all x outside K. Clearly, $C_c(\Omega) \subseteq C_0(\Omega)$, with equality $C_c(\Omega) = C_0(\Omega) = C(\Omega)$ when Ω is compact. Now, when Ω is noncompact it can be shown (by easy examples) that $C_c(\Omega)$ is not complete in the sup-norm; its completion turns out to be $C_0(\Omega)$.

Clearly, $C_c(\Omega)$ lies in the space W of all functions $f : \Omega \to \mathbb{C}$, and according to the above scenario our task is to find a subspace $H \subset W$ that plays the role of the completion of $C_c(\Omega)$ in the norm $\|\cdot\|_2$. There is a complication, however, which does not occur in the case of ℓ^2. Let us ignore this complication first. A detailed study shows that the analogue of ℓ^2 is now given by the space $\mathcal{L}^2(\Omega)$, defined as follows.

Definition II.7 *The space $\mathcal{L}^2(\Omega)$ consists of all functions $f : \Omega \to \mathbb{C}$ for which there exists a Cauchy sequence (f_n) in $C_c(\Omega)$ with respect to $\|\cdot\|_2$ such that $f_n(x) \to f(x)$ for all $x \in \Omega\backslash N$, where $N \subset \Omega$ is a set of (Lebesgue) measure zero.*

Recall (e.g. from [28], p. 110) that a subset $N \subset \mathbb{R}^n$ has measure zero if for any $\epsilon > 0$ there exists a covering of N by an at most countable set (I_n) of intervals for which $\sum_n |I_n| < \epsilon$, where $\sum_n |I_n|$ is the sum of the volumes of the I_n. (Here an interval in $\mathbb{R}^n$ is a set of the form $\prod_{k=1}^n [a_k, b_k]$). For example, any countable subset of $\mathbb{R}^n$ has measure zero, but there are others.

The space $\mathcal{L}^2(\Omega)$ contains all functions f for which $|f|^2$ is Riemann-integrable over Ω (so in particular all of $C_c(\Omega)$, as was already clear from the definition), but many other, much wilder functions. We can extend the inner product on $C_c(\Omega)$ to $\mathcal{L}^2(\Omega)$ by means of

$$(f, g) = \lim_{n\to\infty} (f_n, g_n), \tag{II.12}$$

where (f_n) and (g_n) are Cauchy sequences as specified in the definition of $\mathcal{L}^2(\Omega)$ (see footnote 7).

Consequently (see also footnote 6), taking $g_n = f_n$, the following limit exists:

$$\|f\|_2 := \lim_{n\to\infty} \|f_n\|_2. \tag{II.13}$$

The problem is that (II.12) does not define an inner product on $\mathcal{L}^2(\Omega)$ and that (II.13) does not define a norm on it because these expressions fail to be positive definite. For example, take a function f on $\Omega = [0, 1]$ that is nonzero in finitely (or even countably) many points. The Cauchy sequence with only zeros defines f as an element of $\mathcal{L}^2(\Omega)$, so $\|f\|_2 = 0$ by (II.13), yet $f \neq 0$ as a function. This is related to the following point: the sequence (f_n) does not define f except outside a set of measure zero.

Everything is solved by introducing the space

$$L^2(\Omega) := \mathcal{L}^2(\Omega)/\mathcal{N}, \tag{II.14}$$

where

$$\mathcal{N} := \{f \in \mathcal{L}^2(\Omega) \mid \|f\|_2 = 0.\} \tag{II.15}$$

Using measure theory, it can be shown that $f \in \mathcal{N}$ iff $f(x) = 0$ for all $x \in \Omega\backslash N$, where $N \subset \Omega$ is some set of measure zero. If f is continuous, this implies that $f(x) = 0$ for all $x \in \Omega$.

It is clear that $\|\cdot\|_2$ descends to a norm on $L^2(\Omega)$ by

$$\|[f]\|_2 := \|f\|_2, \tag{II.16}$$

where $[f]$ is the equivalence class of $f \in \mathcal{L}^2(\Omega)$ in the quotient space. However, we normally work with $\mathcal{L}^2(\Omega)$ and regard elements of $L^2(\Omega)$ as functions instead of equivalence classes thereof. So in what follows we should often write $[f] \in L^2(\Omega)$ instead of $f \in \mathcal{L}^2(\Omega)$, but who cares.

We would now like to show that $L^2(\Omega)$ is the completion of $C_c(\Omega)$. The details of the proof require the theory of Lebesgue integration (see [26] or many other books, or the course of A. van Rooij), but the idea is similar to the case of ℓ^2.

Let (f_n) be Cauchy in $\mathcal{L}^2(\Omega)$. By definition of the norm in $L^2(\Omega)$, there is a sequence (h_n) in $C_c(\Omega)$ such that:

1. $\|f_n - h_n\|_2 \leq 2^{-n}$ for all n;
2. $|f_n(x) - h_n(x)| \leq 2^{-n}$ for all $x \in \Omega\backslash A_n$, where $|A_n| \leq 2^{-n}$.

By the first property one can prove that (h_n) is Cauchy, and by the second that $\lim_n h_n(x)$ exists for almost all $x \in \Omega$ (i.e. except perhaps at a set N of measure zero). This limit defines a function $f : \Omega \backslash N \to \mathbb{C}$ for which $h_n(x) \to f(x)$. Outside N, f can be defined in any way one likes. Hence $f \in \mathcal{L}^2(\Omega)$, and its equivalence class $[f]$ in $L^2(\Omega)$ is independent of the value of f on the null set N. It easily follows that $\lim_n f_n = f$ in $\| \cdot \|_2$, so that Cauchy sequence (f_n) converges to an element of $L^2(\Omega)$. Hence $L^2(\Omega)$ is complete.

The identification of $L^2(\Omega)$ with the formal completion of $C_c(\Omega)$ is done in the same way as before: we repeat (II.8), where this time the function $f \in CL^2(\Omega)$ is the one associated to the Cauchy sequence (f_n) in $C_c(\Omega)$ through Definition II.7. As stated before, it would be really correct to write (II.8) as follows:

$$U([f_n]) := [f] = [\lim_n f_n], \tag{II.17}$$

where the square brackets on the left-hand side denote equivalence classes with respect to the equivalence relation $(f_n) \sim (g_n)$ when $\lim_n \|f_n - g_n\|_2 = 0$ between Cauchy sequences in $C_c(\Omega)$, whereas the square brackets on the right-hand side denote equivalence classes with respect to the equivalence relation $f \sim g$ when $\|f - g\|_2 = 0$ between elements of $\mathcal{L}^2(\Omega)$.

We finally note a interesting result about $L^2(\Omega)$ without proof (see [26], Satz 1.41, p. 43):

Theorem II.8 *Every Cauchy sequence (f_n) in $\mathcal{L}^2(\Omega)$ has a subsequence that converges pointwise almost everywhere to some $f \in \mathcal{L}^2(\Omega)$.*

The proof of this theorem yields an alternative approach to the completeness of $L^2(\Omega)$.

In many cases, all you need to know is the following fact about L^2 or $\mathcal{L}^2$, which follows from the fact that $L^2(\Omega)$ is indeed the completion of $C_c(\Omega)$ (and is a consequence of Definition II.7) if enough measure theory is used):

Proposition II.9 *For any $f \in \mathcal{L}^2(\Omega)$ there is a Cauchy sequence (f_k) in $C_c(\Omega)$ such that $f_k \to f$ in norm (i.e. $\lim_{k\to\infty} \|f - f_k\|_2 = 0$).*

Without creating confusion, one can replace $f \in \mathcal{L}^2(\Omega)$ by $f \in L^2(\Omega)$ in this statement, as long as one keeps the formal difference between L^2 and $\mathcal{L}^2$ in the back of one's mind.

II.3 Orthogonality and orthonormal bases

As stressed in the Introduction, Hilbert spaces are the vector spaces whose geometry is closest to that of $\mathbb{R}^3$. In particular, the inner product yields a notion of orthogonality. We say that two vectors $f, g \in H$ are **orthogonal**, written $f \perp g$, when $(f, g) = 0$.[11] Similary, two subspaces[12] $K \subset H$ and $L \subset H$ are said to be orthogonal ($K \perp L$) when $(f, g) = 0$ for all $f \in K$ and all $g \in L$. A vector f is called orthogonal to a subspace K, written $f \perp K$, when $(f, g) = 0$ for all $g \in K$, etc.

For example, if $H = L^2(\Omega)$ and $\Omega = \Omega_1 \cup \Omega_2$, elementary (Riemann) integration theory shows that the following subspaces are orthogonal:[13]

$$K = \{f \in C_c(\Omega) \mid f(x) = 0 \, \forall x \in \Omega_1\}; \tag{II.18}$$

$$L = \{f \in C_c(\Omega) \mid f(x) = 0 \, \forall x \in \Omega_2\}. \tag{II.19}$$

We define the **orthogonal complement** $K^\perp$ of a subspace $K \subset H$ as

$$K^\perp := \{f \in H \mid f \perp K\}. \tag{II.20}$$

This set is automatically linear, so that the map $K \mapsto K^\perp$, called **orthocomplementation**, is an operation from subspaces of H to subspaces of H. Clearly, $H^\perp = 0$ and $0^\perp = H$.

[11] By definition of the norm, if $f \perp g$ one has Pythagoras' theorem $\|f + g\|^2 = \|f\|^2 + \|g\|^2$.

[12] Recall that a subspace of a vector space is by definition a linear subspace.

[13] This may be strengthened as follows: the space K_1 consisting of all $f \in L^2(\Omega)$ that vanish for almost all $x \in \Omega_1$ is orthogonal to the space K_2 consisting of all $f \in L^2(\Omega)$ that vanish for almost all $x \in \Omega_2$. These subspaces are closed in $L^2(\Omega)$, which is not the case for K and L in the main text.

Now, a subspace of a Hilbert space may or may not be closed. A **closed subspace** $K \subset H$ of a Hilbert space H is by definition complete in the given norm on H (i.e. any Cauchy-sequence in K converges to an element of K).[14] This implies that a closed subspace K of a Hilbert space H is itself a Hilbert space if one restricts the inner product from H to K. If K is not closed already, we define its **closure** $\overline{K}$ as the smallest closed subspace of H containing K.[15]

For example, if $\Omega \subset \mathbb{R}^n$ then $C_c(\Omega)$ is a subspace of $L^2(\Omega)$ which is not closed; its closure is $L^2(\Omega)$.[16]

Closure is an analytic concept, related to convergence of sequences. Orthogonality is a geometric concept. However, both are derived from the inner product. Hence one may expect certain connections relating analysis and geometry on Hilbert space.

Proposition II.10 *Let $K \subset H$ be a subspace of a Hilbert space.*

1. *The subspace $K^\perp$ is closed, with*
$$K^\perp = \overline{K}^\perp = \overline{K^\perp}. \tag{II.21}$$
2. *One has*
$$K^{\perp\perp} := (K^\perp)^\perp = \overline{K}. \tag{II.22}$$
3. *Hence for closed subspaces K one has $K^{\perp\perp} = K$.*

The proof is an exercise.

We now turn to the concept of an **orthonormal basis** (o.n.b.) in a Hilbert space. First, one can:

1. Define a Hilbert space H to be **finite-dimensional** if has a finite o.n.b. (e_k) in the sense that $(e_k, e_l) = \delta_{kl}$ and any $v \in H$ can be written as $v = \sum_k v_k e_k$ for some $v_k \in \mathbb{C}$;
2. Prove (by elementary linear algebra) that any o.n.b. in a finite-dimensional Hilbert space H has the same cardinality;
3. Define the dimension of H as the cardinality of an arbitary o.n.b. of H.

It is trivial to show that if $v = \sum_k v_k e_k$, then
$$v_k = (e_k, v) \tag{II.23}$$
and
$$\sum_k |(e_k, v)|^2 = \|v\|^2. \tag{II.24}$$
This is called **Parseval's equality**; it is a generalization of Pythagoras's Theorem. Note that if H is finite-dimensional, then any subspace is (automatically) closed (exercise).

Now what happens when H is not finite-dimensional? In that case, it is called **infinite-dimensional**. The spaces ℓ^2 and $L^2(\Omega)$ are examples of infinite-dimensional Hilbert spaces. We call an infinite-dimensional Hilbert space **separable** when it contains a *countable* orthonormal set $(e_k)_{k\in\mathbb{N}}$ such that any $v \in H$ can be written as
$$v = \sum_{k=1}^{\infty} v_k e_k \tag{II.25}$$

[14] Since H is a Hilbert space we know that the sequence has a limit in H, but this limit may not lie in K even when all elements of the sequence lie in K. This possibility arises precisely when K fails to be closed.

[15] This closure is isomorphic to the abstract completion of K as explained before.

[16] More precisely, as we have seen $C_c(\Omega)$ is really a subspace of $\mathcal{L}^2(\Omega)$, so what is meant here is that the collection of equivalence classes of functions in $C_c(\Omega)$ is a non-closed subspace of $L^2(\Omega)$. But notations such as $C_c(\Omega) \subset L^2(\Omega)$, though strictly speaking false, are not misleading and will often be used in what follows. In fact, if $f \in C_c(\Omega)$ then the equivalence class $[f] \in L^2(\Omega)$ contains a unique element that is continuous, namely f itself!

for some $v_k \in \mathbb{C}$. By definition, this means that

$$v = \lim_{N\to\infty} \sum_{k=1}^{N} v_k e_k \tag{II.26}$$

where the limit means that

$$\lim_{N\to\infty} \|v - \sum_{k=1}^{N} v_k e_k\| = 0. \tag{II.27}$$

Here the norm is derived from the inner product in the usual way. Such a set is again called an **orthonormal basis**. It is often convenient to take $\mathbb{Z}$ instead of $\mathbb{N}$ as the index set of the basis, so that one has $(e_k)_{k\in\mathbb{Z}}$ and

$$v = \lim_{N\to\infty} \sum_{k=-N}^{N} v_k e_k. \tag{II.28}$$

It is an exercise to show that (II.23) and (II.24) are still valid in the infinite-dimensional case. Also, the following lemma will often be used:

Lemma II.11 *Let (e_k) be an o.n.b. in an infinite-dimensional separable Hilbert space H and let $f, g \in H$. Then*

$$\sum_k (f, e_k)(e_k, g) = (f, g). \tag{II.29}$$

This follows if one expands f and g on the right-hand side according to (II.25) and uses (II.23); one has to be a little bit careful with the infinite sums but these complications are handled in the same way as in the proof of (II.23) and (II.24).

The following result is spectacular:[17]

Theorem II.12 *1. Two finite-dimensional Hilbert spaces are isomorphic iff they have the same dimension.*

2. Any two separable infinite-dimensional Hilbert spaces are isomorphic.

The proof, though, is left as an exercise. It relies on the choice of a basis in each of the two spaces under consideration. To illustrate the theorem, we show that $\ell^2(\mathbb{Z})$ and $L^2([-\pi, \pi])$ are isomorphic through the Fourier transform. Namely, using Fourier theory (see [28]) one can show that the functions $(e_k)_{k\in\mathbb{Z}}$ defined by

$$e_k(x) := \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{II.30}$$

from an o.n.b. of $L^2([-\pi, \pi])$. Trivially, the functions $(\varphi_k)_{k\in\mathbb{Z}}$ defined by

$$\varphi_k(l) := \delta_{kl} \tag{II.31}$$

form an o.n.b of $\ell^2(\mathbb{Z})$. (If one regards an element of $\ell^2(\mathbb{Z})$ as a sequence instead of a function, f_k is the sequence with a 1 at position k and zero's everywhere else.) This shows that $\ell^2(\mathbb{Z})$ and $L^2([-\pi, \pi])$ are both separable infinite-dimensional, and hence isomorphic by Theorem II.12. Indeed, it is trivial to write down the unitary map $U : L^2([-\pi, \pi]) \to \ell^2(\mathbb{Z})$ that 'makes' $\ell^2(\mathbb{Z})$ and $L^2([-\pi, \pi])$ isomorphic according to the definition of isomorphism: one simply puts

$$Uf(k) := (e_k, f)_{L^2} = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dx\, e^{-ikx} f(x). \tag{II.32}$$

[17] The general statement is as follows. One can introduce the notion of an orthonormal basis for an arbitrary Hilbert space as a maximal orthonormal set (i.e. a set of orthonormal vectors that is not properly contained in any other orthonormal set). It is an exercise to show that in the separable case, this notion of a basis is equivalent to the one introduced in the main text. One then proves that any two orthonormal bases of a given Hilbert space have the same cardinality. Hence one may define the dimension of a Hilbert space as the cardinality of an arbitrary orthonormal basis. Theorem II.12 then reads in full glory: *Two Hilbert spaces are isomorphic iff they have the same dimension.* See [18].

Here $f \in \mathcal{L}([-\pi,\pi])$. The second equality comes from the definition of the inner product in $L^2([-\pi,\pi])$. The inverse of U is $V : \ell^2(\mathbb{Z}) \to L^2([-\pi,\pi])$, given by

$$V\varphi := \sum_{k\in\mathbb{Z}} \varphi(k) e_k, \tag{II.33}$$

where $\varphi \in \ell^2(\mathbb{Z})$. It is instructive to verify that $V = U^{-1}$:

$$(UV\varphi)(k) = (e_k, V\varphi)_{L^2} = (e_k, \sum_l \varphi(l) e_l)_{L^2} = \sum_l \varphi(l)(e_k, e_l)_{L^2} = \sum_l \varphi(l)\delta_{kl} = \varphi(k),$$

where one justifies taking the infinite sum over l out of the inner product by the Cauchy-Schwarz inequality (using the fact that $\sum_l \|\varphi(l)\|^2 < \infty$, since by assumption $\varphi \in \ell^2(\mathbb{Z})$). Similarly, for $f \in L^2([-\pi,\pi])$ one computes

$$VUf = \sum_k (Uf)(k) e_k = \sum_k (e_k, f)_{L^2} e_k = f$$

by (II.25) and (II.23). Of course, all the work is in showing *that* the functions e_k form an o.n.b. of $L^2([-\pi,\pi])$, which we have not done here!

Hence $V = U^{-1}$, so that (II.33) reads

$$U^{-1}\varphi(x) = \sum_{k\in\mathbb{Z}} \varphi(k) e_k(x) = \frac{1}{\sqrt{2\pi}} \sum_{k\in\mathbb{Z}} \varphi(k) e^{ikx}. \tag{II.34}$$

Finally, the unitarity of U follows from the computation (where $f, g \in L^2$)

$$(Uf, Ug)_{\ell^2} = \sum_k (f, e_k)_{L^2} (e_k, g)_{L^2} = (f, g)_{L^2},$$

where we have used (II.29).

The choice of a basis in the argument that $\ell^2(\mathbb{Z}) \cong L^2([-\pi,\pi])$ was clearly essential. There are pairs of concrete Hilbert spaces, however, which one can show to be isomorphic *without choosing bases*. A good example is provided by (II.8) and surrounding text, which proves the "practical" completion ℓ^2 of ℓ_c and the formal completion $\tilde{\ell}_c$ to be isomorphic. If one can find a unitary map $U : H_1 \to H_2$ without choosing bases, the two Hilbert spaces in question are called **naturally isomorphic**. As another example, the formal completion $\widetilde{C_c(\Omega)}$ of $C_c(\Omega)$ is naturally isomorphic to $L^2(\Omega)$.

Chapter III

Operators and functionals

III.1 Bounded operators

For the moment, we are finished with the description of Hilbert spaces on their own. Indeed, Theorem II.12 shows that, taken by themselves, Hilbert spaces are quite boring. The subject comes alive when one studies operators on Hilbert spaces. Here an **operator** $a : H_1 \to H_2$ between two Hilbert space is nothing but a linear map (i.e., $a(\lambda v + \mu w) = \lambda a(v) + \mu a(w)$ for all $\lambda, \mu \in \mathbb{C}$ and $v, w \in H_1$). We usually write av for $a(v)$.

The following two special cases will occur time and again:

1. Let $H_1 = H$ and $H_2 = \mathbb{C}$: a linear map $\varphi : H \to \mathbb{C}$ is called a **functional** on H.
2. Let $H_1 = H_1 = H$: a linear map $a : H \to H$ is just called an operator on H.

To construct an example of a functional on H, take $f \in H$ and define $\varphi_f : H \to \mathbb{C}$ by

$$\varphi_f(g) := (f, g). \tag{III.1}$$

When H is finite-dimensional, any operator on H can be represented by a matrix and the theory reduces to linear algebra. For an infinite-dimensional example, take $H = \ell^2$ and $\hat{a} \in \ell^\infty$. It is an exercise to show that if $f \in \ell^2$, then $\hat{a}f \in \ell^2$. Hence may define an operator $a : \ell^2 \to \ell^2$ by

$$\hat{a}f := af. \tag{III.2}$$

We will often write a for this operator instead of $\hat{a}$. Similarly, take $H = L^2(\Omega)$ and $\hat{a} \in C_b(\Omega)$ (where $C_b(\Omega)$ is the space of bounded continuous functions on $\Omega \subset \mathbb{R}^n$, i.e. $\hat{a} : \Omega \to \mathbb{C}$ is continuous and $\|\hat{a}\|_\infty < \infty$). As in the previous example, it is an exercise to show that if $f \in L^2(\Omega)$ and $\hat{a} \in C_b(\Omega)$, then $\hat{a}f \in L^2(\Omega)$.[1] Thus also in this case (III.2) defines an operator $a : L^2(\Omega) \to L^2(\Omega)$, called a **multiplication operator**.

Finally, the operators U and V constucted at the end of the previous chapter in the context of the Fourier transform give examples of operators between different Hilbert spaces.

As in elementary analysis, where one deals with functions $f : \mathbb{R} \to \mathbb{R}$, it turns out to be useful to single out functions with good properties, notably continuity. So what does one mean by a 'continuous' operator $a : H_1 \to H_2$? One answer come from topology: the inner product on a Hilbert space defines a norm, the norm defines a metric, and finally the metric defines a topology, so one may use the usual definition of a continuous function $f : X \to Y$ between two topological spaces.[2] Since we do not require students of this course to be familiar with abstract topology, we use another definition, which turns out to be equivalent to the topological one. (In fact, the definition below is much more useful than the topological definition.)

[1] The easiest way to do this exercise is to start with $f \in C_c(\Omega)$; the fact that $\hat{a}f \in L^2(\Omega)$ then follows from an elementary estimate from Riemann integration theory. One then passes to the general case by an approximation argument using Proposition II.9.

[2] Recall that f is called continuous when $f^{-1}(\mathcal{O})$ is open in X for any open set $\mathcal{O}$ in Y.

Definition III.1 *$a : H_1 \to H_2$ be an operator. Define a positive number $\|a\|$ by*

$$\|a\| := \sup\{\|av\|_{H_2},\, v \in H_1,\, \|v\|_{H_1} = 1\}, \tag{III.3}$$

where $\|v\|_{H_1} = \sqrt{(v,v)_{H_1}}$, etc. We say that a is **continuous** *or* **bounded** *when $\|a\| < \infty$.*

For the benefit of those familiar with topology, we mention without proof that a is continuous according to this definition iff it is continuous in the topological sense, as explained above. This may be restated as follows: an operator $a : H_1 \to H_2$ is continuous (in the topological sense) iff it is bounded (in the sense of Definition III.1).

Geometrically, the set $\{v \in H_1,\, \|v\|_{H_1} = 1\}$ is the unit ball in H_1, i.e. the set of vectors of length 1 in H_1. Hence $\|a\|$ is the supremum of the function $v \mapsto \|av\|_{H_2}$ from the unit ball in H_1 to $\mathbb{R}^+$. If H_1 is finite-dimensional the unit ball in H_1 is compact. Since the function just mentioned is continuous, it follows that any operator a on a finite-dimensional Hilbert space is bounded (as a continuous function from a compact set in $\mathbb{R}^n$ to $\mathbb{R}$ assumes a maximum somewhere).[3]

If a is bounded, the number $\|a\|$ is called the **norm** of a. This terminology remains to be justified; for the moment it is just a name. It is easy to see that if $\|a\| < \infty$, the norm of a coincided with the constant

$$\|a\| = \inf\{C \geq 0 \mid \|av\|_{H_2} \leq C\|v\|_{H_1}\ \forall v \in H_1\}. \tag{III.4}$$

Moreover, if a is bounded, then it is immediate that

$$\|av\|_{H_2} \;\leq\; \|a\|\,\|v\|_{H_1} \tag{III.5}$$

for all $v \in H_1$. This inequality is very important. For example, it trivially implies that

$$\|ab\| \leq \|a\|\|b\|, \tag{III.6}$$

where $a : H \to H$ and $b : H \to H$ are any two bounded operators, and $ab := a \circ b$, so that $(ab)(v) := a(bv)$.

In the examples just considered, all operators turn out to be bounded. First take a functional $\varphi : H \to \mathbb{C}$; since $\|\cdot\|_{\mathbb{C}} = |\cdot|$, one has

$$\|\varphi\| := \sup\{|\varphi(v)|,\, v \in H,\, \|v\|_H = 1\}. \tag{III.7}$$

If one uses Cauchy–Schwarz, it is clear from (III.1) that $\|\varphi_f\| \leq \|f\|_H$. In fact, an important result in Hilbert space theory says:

Theorem III.2 *Let H be a Hilbert space. Any functional of the form φ_f for some $f \in H$ (see* (III.1)*) is continuous. Conversely, any continuous functional $\varphi : H \to \mathbb{C}$ is of the form $\varphi_f : g \mapsto (f,g)$ for some unique $f \in H$, and one has*

$$\|\varphi_f\| = \|f\|_H. \tag{III.8}$$

The proof is as follows. First, given $f \in H$, as already mentioned, φ_f is bounded by Cauchy–Schwarz. Conversely, take a continuous functional $\varphi : H \to \mathbb{C}$, and let N be the kernel of φ. This is a closed subspace of H by the boundedness of φ. If $N = H$ then $\varphi = 0$ so we are ready, since $\varphi = \varphi_{f=0}$. Assume $N \neq H$. Since N is closed, $N^\perp$ is not empty, and contains a vector h with $\|h\| = 1$.[4] For any $g \in H$, one has $\varphi(g)h - \varphi(h)g \in N$, so $(h, \varphi(g)h - \varphi(h)g) = 0$, which means $\varphi(g)(h,h) = \varphi(h)(h,g)$, or $\varphi(g) = (f,g)$ with $f = \overline{\varphi(h)}h$.

To prove uniqueness of f, suppose there is h' with $h' \in \ker(\varphi)^\perp$ and $\|h'\| = 1$, and consequently also $\varphi(g) = (f',g)$ with $f' = \overline{\varphi(h')}h'$. Then $\varphi(h) = \varphi(h')(h',h)$, so that $h - (h',h)h' \in \ker(\varphi)$.

[3] If $a : \mathbb{C}^n \to \mathbb{C}^n$ is linear, can be shown from the minimax-property of eigenvalues that $\|a\|^2$ coincides with the largest eigenvalue of a^*a.

[4] To see this, pick an orthonormal basis (e_n) of N. Since N is closed, any f of the form $f = \sum_n c_n e_n$, $c_n \in \mathbb{C}$, that lies in H (which is the case iff $\sum_n |c_n|^2 < \infty$) actually lies in N. Since $N \neq H$, there exists $g \notin N$, which implies that $g \neq \sum_n (e_n, g)e_n$, or $h := g - \sum_n (e_n, g)e_n \neq 0$. Clearly, $h \in N^\perp$, and since $h \neq 0$ the vector $h/\|h\|$ has norm 1. This argument will become clearer after the introduction of projections later in this chapter.

But $\ker(\varphi)^\perp$ is a linear subspace of H, so it must be that $h - (h', h)h' \in \ker(\varphi)^\perp$ as well. Since $\ker(\varphi)^\perp \cap \ker(\varphi) = 0$, it follows that $h - (h', h)h' = 0$. Hence $h = (h', h)h'$ and therefore $\|h'\| = 1$ and $\|h\| = 1$ yield $|(h, h')| = 1$, or $\overline{(h', h)}(h', h) = 1$. It follows that

$$f = \overline{\varphi(h)}h = \overline{(h', h)\varphi(h')}(h', h)h' = \overline{\varphi(h')}h' = f'.$$

To compute $\|\varphi_f\|$, first use Cauchy–Schwarz to prove $\|\varphi_f\| \leq \|f\|$, and then apply φ_f to f to prove equality. ∎

For an example of a bounded operator $a : H \to H$, note that on ℓ^2 as well as on $L^2(\Omega)$ the operator $\hat{a}$ defined by (III.2) is bounded, with

$$\|a\| = \|\hat{a}\|_\infty. \tag{III.9}$$

The proof of this result is an exercise. This exercise involves the useful estimate

$$\|af\|_2 \leq \|\hat{a}\|_\infty \|f\|_2, \tag{III.10}$$

which in turn follows from (III.9) (supposing one already knew this) and (III.5).

Finally, the operators U and V at the end of the previous chapter are unitary; it easily follows from the definition of unitarity that

$$\|U\| = 1 \tag{III.11}$$

for any unitary operator U.

What about discontinuous or unbounded operators? In view of (III.9), let us take an unbounded function $\hat{a} : \mathbb{Z} \to \mathbb{C}$ and attempt to define an operator $a : \ell^2 \to \ell^2$ by means of (III.2), hoping that $\|a\| = \infty$. The problem with this attempt is that in fact an unbounded function does *not* define a map from ℓ^2 to ℓ^2 at all, since $\hat{a}f$ will not be in ℓ^2 for many choices of $f \in \ell^2$. (For example, consider $\hat{a}(k) = k$ and find such an f for which $\hat{a}f \notin \ell^2$ yourself.) This problem is generic: as soon as one has a candidate for an unbounded operator $a : H_1 \to H_2$, one discovers that in fact a does not map H_1 into H_2.

Nonetheless, unbounded operators occur naturally in many examples and hence are extremely important in practice, especially in quantum mechanics and the theory of (partial) differential equations. But they are not constructed in the above manner as maps from H_1 to H_2. To prepare for the right concept of an unbounded operator, let us look at the bounded case once more. We restrict ourselves to the case $H_1 = H_2 = H$, as this is the relevant case for quantum mechanics.

As before, we denote the completion or closure of a subspace D of a Hilbert space H by $\overline{D} \subset V$.

Proposition III.3 *Let $D \subset H$ be a subspace of a Hilbert space, and let $a : D \to H$ be a linear map. Define the positive number*

$$\|a\|_D := \sup\{\|av\|_H,\ v \in D,\ \|v\|_H = 1\}. \tag{III.12}$$

If $\|a\|_D < \infty$, there exists a unique bounded extension of a to an operator $a^- : \overline{D} \to H$ with

$$\|a^-\| = \|a\|_D. \tag{III.13}$$

In particular, when D is dense in H (in the sense that $\overline{D} = H$), the extension a^- is a bounded operator from H to H.

Conversely, a bounded operator $a : H \to H$ is determined by its restriction to a dense subspace $D \subset H$.

The proof is an exercise. The idea is to define a^-v for $v \notin D$ by $a^-v := \lim_n av_n$, where $(v_n) \subset D$ converges to v. We leave the easy details to the reader. Hence in the above examples it suffices to compute the norm of a in order to find the norm of a^-.

The point is now that unbounded operators are defined as linear maps $a : D \to H$ for which $\|a\|_D = \infty$. For example, take $\hat{a} \notin \ell^\infty$ and $f \in D = \ell_c$. Then $af = \hat{a}f \in \ell_c$, so that $a : \ell_c \to \ell^2$ is defined. It is an exercise to show that $\|a\|_{\ell_c} = \infty$ iff $\hat{a} \notin \ell^\infty$ (i.e. $\hat{a}$ is unbounded). Another example is $af := df/dx$, defined on $f \in C^{(1)}([0,1]) \subset L^2([0,1])$. Once again, it is an exercise to show that $\|d/dx\|_{C^{(1)}([0,1])} = \infty$. In quantum mechanics, operators like position, momentum and the Hamiltonian of a particle in a potential are unbounded (see exercises).

III.2 The adjoint

Now let H be a Hilbert space, and let $a : H \to H$ be a bounded operator. The inner product on H gives rise to a map $a \mapsto a^*$, which is familiar from linear algebra: if $H = \mathbb{C}^n$, so that, upon choosing the standard basis (e_i), a is a matrix $a = (a_{ij})$ with $a_{ij} = (e_i, ae_j)$, then the adjoint is given by $a^* = (\overline{a_{ji}})$. In other words, one has

$$(a^* f, g) = (f, ag) \tag{III.14}$$

for all $f, g \in \mathbb{C}^n$. This equation defines the adjoint also in the general case, but to prove existence of a^* Theorem III.8 is needed: for fixed $a \in B(H)$ and $f \in H$, one defines a functional $\varphi_f^a : H \to \mathbb{C}$ by $\varphi_f^a(g) := (f, ag)$. This functional is bounded by Cauchy–Schwarz and (III.5):

$$|\varphi_f^a(g)| = |(f, ag)| \leq \|f\|\|ag\| \leq \|f\|\|a\|\|g\|,$$

so $\|\varphi_f^a\| \leq \|f\|\|a\|$. Hence by Theorem III.8 there exists a unique $h \in H$ such that $\varphi_f^a(g) = (h, g)$ for all $g \in H$. Now, for given a the association $f \mapsto h$ is clearly linear, so that we may define $a^* : H \to H$ by $a^* f := h$; eq. (III.14) then trivially follows. Note that the map $a \mapsto a^*$ is anti-linear: one has $(\lambda a)^* = \overline{\lambda} a$ for $\lambda \in \mathbb{C}$.

It is an exercise to show that for each $a \in B(H)$ one has

$$\|a^*\| = \|a\|; \tag{III.15}$$

$$\|a^* a\| = \|a\|^2. \tag{III.16}$$

A bounded operator $a : H \to H$ is called **self-adjoint**[5] when $a^* = a$. It immediately follows form (III.14) that for self-adjoint a one has $(f, af) \in \mathbb{R}$.[6]

One may also define self-adjointness in the unbounded case, in a way very similar to the story above. Namely, let $D \subset H$ be dense and let $a : D \to H$ be a possibly unbounded operator. We write $D(a)$ for D and define an operator $a^* : D(a^*) \to H$ as follows.

Definition III.4 *1. The adjoint a^* of an unbounded operator $a : D(a) \to H$ has domain $D(a^*)$ consisting of all $f \in H$ for which the functional $g \mapsto \varphi_f^a(g) := (f, ag)$ is bounded. On this domain, a^* is defined by requiring $(a^* f, g) = (f, ag)$ for all $g \in D(a)$.*

2. The operator a is called **self-adjoint** *when $D(a^*) = D(a)$ and $a^* = a$.*

Here the vector $a^* f$ once again exists by the Theorem III.8 (indeed, the definition has been formulated precisely so as to guarantee that $a^* f$ exists!), and it is uniquely determined by our assumption that $D(a)$ be dense in H. However, this time we cannot conclude that $D(a^*) = H$, as in the bounded case. Indeed, it may even happen that $D(a^*)$ is zero! However, this is pretty pathological, and in most 'natural' examples $D(a^*)$ turns out to be dense. For example, a multiplication operator $\hat{a} \in C(\Omega)$ on $H = L^2(\Omega)$, defined on the domain $D(a) = C_c(\Omega)$ by $af = \hat{a} f$ as usual, has $a^* = \overline{a}$ (i.e., the complex conjugate of a seen as a multiplication operator) defined on the domain $D(a^*)$ given by

$$D(a^*) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}. \tag{III.17}$$

Since $D(a) \subset D(a^*)$, the operator a cannot be self-adjoint. However, if we start again and define a on the domain specified by the right-hand side of (III.17), it turns out that this time one does have $a^* = a$. We will study such questions in detail later on, as they are very important for quantum mechanics.

We return to the bounded case.

[5] Or **Hermitian**.

[6] In quantum mechanics self-adjoint operators model physical observables, so that these have real expectation values.

III.3 Projections

The most important examples of self-adjoint operators are projections.

Definition III.5 *A* **projection** *on a Hilbert space H is a bounded operator $p \in B(H)$ satisfying $p^2 = p^* = p$.*

To understand the significance of projections, the reader should first recall the discussion about orthogonality and bases in Hilbert spaces in Chapter II.II.3. Now let $K \subset H$ be a closed subspace of H; such a subspace is a Hilbert space by itself, and therefore has an orthonormal basis (e_i). Applying (II.25) with (II.23) to K, it is easy to verify that

$$p : f \mapsto \sum_i (e_i, f) e_i \tag{III.18}$$

for each $f \in H$, where the sum converges in H,[7] defines a projection. Clearly,

$$\begin{aligned} pf &= f \quad \text{for } f \in K; \\ pf &= 0 \quad \text{for } f \in K^\perp. \end{aligned} \tag{III.19}$$

Proposition III.6 *For each closed subspace $K \subset H$ one has $H = K \oplus K^\perp$. In other words, given any closed subspace $K \subset H$ each $f \in H$ has a unique decomposition $f = f^\parallel + f^\perp$, where $f^\parallel \in K$ and $f^\perp \in K^\perp$.*

The existence of the decomposition is given by $f^\parallel = pf$ and $f^\perp = (1-p)f$, and its uniqueness follows by assuming $f = g^\parallel + g^\perp$ with $g^\parallel \in K$ and $g^\perp \in K^\perp$: one then has $f^\parallel - g^\parallel = f^\perp - g^\perp$, but since the left-hand side is in K and the right-hand side is in $K^\perp$, both sides lie in $K \cap K^\perp = 0$. ■

Conversely, given a projection p, define $K := pH$. This is a closed subspace of H: if $f \in pH$ then $f = pg$ for some $g \in H$, but then $pf = p^2 g = pg = f$, so that $f \in pH$ iff $pf = f$. If $f_n \to f$ for $f_n \in pH$, then $pf = \lim_n pf_n = \lim f_n = f$, hence $f \in pH$. Furthermore, $K^\perp = (1-p)H$; verifying this fact uses both $p^* = p$ and $p^2 = p$. Defining $f^\parallel := pf$ and $f^\perp := (1-p)f$, one clearly has $f = f^\parallel + f^\perp$ with $f^\parallel \in K$ and $f^\perp \in K^\perp$, so this is the unique decomposition of f described in Proposition III.6. Hence $f^\parallel$ is given, for arbitrary $f \in H$, by both the right-hand side of (III.18) and by pf, so that (III.18) holds and p is completely characterized by its image. Hence we have proved:

Theorem III.7 *There is a bijective correspondence $p \leftrightarrow K$ between projections p on H and closed subspaces K of H: given a projection p one puts $K := pH$, and given a closed subspace $K \subset H$ one defines p by (III.18), where (e_i) is an arbitrary orthonormal basis of K.*

An important special case of a projection is the unit operator $p = 1$, associated with $K = H$.

Projections are important in many ways. One is their occurrence in the spectral theorem, which will occupy us for the remainder of the course. For the moment, let us mention that the spectral theorem of linear algebra has an elegant reformulation in terms of projections. In the usual formulation, a matrix $a : \mathbb{C}^n \to \mathbb{C}^n$ satisfying $a^* a = a a^*$ has an o.n.b. of eigenvectors $\{e_i\}_{i=1,\ldots,n}$, i.e. one has $ae_i = \lambda_i e_i$ for some $\lambda_i \in \mathbb{C}$. In the list of eigenvalues $\{\lambda_i\}_{i=1,\ldots,n}$, some may coincide. Now make a list $\{\lambda_\alpha\}_{\alpha=1,\ldots,m\leq n}$ where all the λ_α's are different. Let p_α be the projection onto the subspace $H_\alpha = p_\alpha \mathbb{C}^n$ of all $f \in \mathbb{C}^n$ for which $af = \lambda_\alpha f$; of course, H_α is the linear span of those e_i for which $\lambda_\alpha = \lambda_i$. The spectral theorem now states that $a = \sum_\alpha \lambda_\alpha p_\alpha$. In other words, each normal matrix is a linear combination of mutually orthogonal projections. We will see in due course what remains of this theorem if one passes from $\mathbb{C}^n$ to an arbitrary (separable) Hilbert space.

Furthermore, it follows from Proposition III.6 that $f \in H$ is an eigenvector of p iff $f \in pH$ or $f \in (pH)^\perp$; in the first case the eigenvector is 1, and in the second case it is 0.

[7] The sum does not converge in the operator norm unless it is finite.

Apart from projections, another important class of operators on a Hilbert space consists of the unitaries. An operator $u : H \to H$ is called **unitary** when $uu^* = u^*u = 1$. Equivalently, u is **isometric**, in that $(uf, uf) = (f, f)$ for all $f \in H$, and invertible (with inverse $u^{-1} = u^*$). For example, if (e_i) and (u_i) are two orthonormal bases of H, then the operator $u(\sum_i c_i e_i) := \sum_i c_i u_i$ is unitary. In quantum mechanics, one usually encounters unitary operators of the form $u = \exp(ia)$, where a is self-adjoint and (for bounded a) the exponential is defined by its usual power series expansion, which converges in operator norm. Clearly, one has $u^* = \exp(-ia)$ and since for commuting a and b (that is, $ab = ba$) one has $\exp(a + b) = \exp(a)\exp(b)$, one sees immediately that u is indeed unitary.[8]

A **partial isometry** is an operator v for which $v^*v = p$ is a projection. A special case is an **isometry**, characterized by $p = 1$, i.e., $v^*v = 1$. An invertible isometry is clearly unitary. The structure of partial isometries is as follows.

Proposition III.8 *If v is a partial isometry, then v^* is a partial isometry as well. Let the associated projection be $q := vv^*$. The kernel of v is $(pH)^\perp$, and its range is qH. The operator v is unitary from pH to its range qH and zero on $(pH)^\perp$. Conversely, any partial isometry has this form for projections p and q.*

The proof is an exercise.

[8] In quantum mechanics the operator a is generally unbounded, a case we will deal with in great detail later on.

Chapter IV

Compact operators

IV.1 Linear algebra revisited

Compact operators on a Hilbert space (or, more generally, on a Banach space) are special bounded operators that behave like matrices on $\mathbb{C}^n$ in many ways. To make this point, we first recall the proof that any hermitian matrix (a_{ij}) (i.e., satisfying $\overline{a_{ji}} = a_{ij}$) can be diagonalized. In linear algebra this theorem is usually stated in a basis-dependent form. From our more abstract perspective of operators, the matrix (a_{ij}) arises from the operator $a : \mathbb{C}^n \to \mathbb{C}^n$ through the choice of an arbitrary orthonormal basis (e_i), in terms of which one has $a_{ij} = (e_i, ae_j)$. The spectral theorem then states that $\mathbb{C}^n$ has a (possibly) new basis of eigenvectors (u_i), in which a is diagonal: with respect to this basis one has $\tilde{a}_{ij} = (u_i, au_j) = (u_i, \lambda_j u_j) = \lambda_i \delta_{ij}$, where λ_i are the eigenvalues of a (possibly degenerate). Now, this result can be restated without any reference to the notion of a basis, as follows.

Proposition IV.1 *Let $H = \mathbb{C}^n$ be a finite-dimensional Hilbert space, and let Let $a : H \to H$ be a self-adjoint operator on H. There exists a family of mutually orthogonal projections (p_α) (i.e., $p_\alpha H \perp p_\beta H$ for $\alpha \neq \beta$, or $p_\alpha p_\beta = \delta_{\alpha\beta}$) with $\sum_\alpha p_\alpha = 1$ and $a = \sum_\alpha \lambda_\alpha p_\alpha$, where λ_α are the eigenvalues of a. In other words, p_α is the projection onto the eigenspace in H with eigenvalue λ_α; the dimension of $p_\alpha H$ is equal to the multiplicity of the eigenvalue λ_α.*

The key to the proof is the following lemma.

Lemma IV.2 *Every self-adjoint operator a on $H = \mathbb{C}^n$ has an eigenvector with associated eigenvalue λ satisfying $|\lambda| = \|a\|$.*

Note that by definition of the operator norm an eigenvalue cannot possibly be any bigger!

The proof uses some topology, but in the restricted context of $H = \mathbb{C}^n$ we simply say (Heine–Borel) that a set is compact when it is closed and bounded. We will use the following facts:

Lemma IV.3 *1. The image of a compact set in H under a continuous map into H or $\mathbb{C}$ is compact.*[1]

2. A continuous function $f : K \to \mathbb{R}$ on a compact set K attains a maximum and a minimum.

We now prove Lemma IV.2. First, the unit ball $B_1 \subset H$, defined in general by

$$B_1 := \{f \in H \mid \|f\| \leq 1\}, \tag{IV.1}$$

is clearly compact in $H = \mathbb{C}^n$. We know from basic analysis that any linear map $a : \mathbb{C}^n \to \mathbb{C}^n$ is continuous,[2] so that aB_1 is compact as well. The norm $f \mapsto \|f\|$ is continuous on H, hence

[1] This true in general: if $f : K \to Y$ is a continuous map between a compact space K and an arbitrary topological space Y, then $f(K)$ is compact in Y.

[2] A linear map $V \to V$ on a normed vector space is continuous iff it is continuous at zero. The latter easily follows for $V = \mathbb{C}^n$. The map is therefore bounded by definition (cf. (III.3)).

it follows that the function $f \mapsto \|af\|^2$ attains a maximum on B_1, say at $f = f_0$, obviously with $\|f_0\| = 1$. By definition of the norm (cf. (III.3)), this maximum must be $\|a\|^2$, so that $\|a\|^2 = \|af_0\|^2$. Cauchy–Schwarz and $a^* = a$ then yield

$$\|a\|^2 = \|af_0\|^2 = (af_0, af_0) = (f_0, a^2 f_0) \leq \|f_0\|\|a^2 f_0\| \leq \|a^2\| = \|a\|^2,$$

where we have used (III.16). In the Cauchy–Schwarz inequality (I.5) one has equality iff $g = zf$ for some $z \in \mathbb{C}$, so that we must have $a^2 f_0 = zf_0$, with $|z| = \|a\|^2$. Moreover, $z \in \mathbb{R}$, as for any self-adjoint operator eigenvalues must be real (trivial exercise!), so $a^2 f_0 = \lambda^2 f_0$ with either $\lambda = \|a\|$ or $\lambda = -\|a\|$. Now either $af_0 = \lambda f_0$, in which case the lemma is proved, or $g_0 := af_0 - \lambda f_0 \neq 0$. In the latter case,

$$ag_0 = a^2 f_0 - \lambda a f_0 = \lambda^2 f_0 - \lambda a f_0 = -\lambda g_0,$$

and the lemma follows, too. ■

Given this lemma, the proof of Proposition IV.1 is peanuts. If $(g, f_0) = 0$ then

$$(ag, f_0) = (g, a^* f_0) = (g, af_0) = \pm\lambda(g, f_0) = 0,$$

so that a maps $f_0^\perp$ into itself. In other words, if p is the projection onto $f_0^\perp$ then $pa = ap$ and $pa = pap$ is the restriction of a to $f_0^\perp = pH$. We now iterate the above procedure: we apply exactly the same reasoning to pa as an operator on pH, finding an eigenvector f_1 of pa, which of course is an eigenvector of a, as $a = pa$ on pH. We then form the orthogonal complement of f_1 in pH, etcetera. Since H is finite-dimensional, this procedure ends after n steps, leaving us with a basis $\{f_0, \ldots, f_{n-1}\}$ of H that entirely consists of eigenvectors by construction. Finally, we assemble those eigenvectors f_k with the same eigenvalue λ_α and define p_α to be the projection onto their linear span K_α (i.e., p_α is given by (III.18) applied to $K = K_\alpha$). ■

IV.2 The spectral theorem for self-adjoint compact operators

Let H be infinite-dimensional (and separable).[3] Eigenvectors and eigenvalues of operators a on a Hilbert space H are defined in the same way as for $H = \mathbb{C}^n$: if $af = \lambda f$ for some $\lambda \in \mathbb{C}$ then $f \in H$ is called an eigenvector of a with eigenvalue λ. A crucial difference with the finite- dimensional situation is that even a bounded self-adjoint operator on an infinite-dimensional Hilbert space may not have any eigenvectors (let alone a basis of them!). For example, on $H = L^2(\Omega)$ a multiplication operator defined by a nonzero continuous function has no eigenfunctions at all. The idea is now to define a class of operators on H for which the proof of Proposition IV.1 can be copied, so that the existence of a complete set of eigenvectors is guaranteed.

We will once again need some topology, but in our setting of separable Hilbert spaces we may keeps things simple: a set K in a separable Hilbert space H is **compact** when every sequence in K has a convergent subsequence, and a map $\alpha : H \to T$, where $T = \mathbb{C}$ or $T = H$, is **continuous** if it "preserves limits," i.e., if $f_n \to f$ in H then $\alpha(f_n) \to \alpha(f)$ in T.[4] For $H = \mathbb{C}^n$, this notion of compactness is equivalent to the Heine–Borel property; for separable infinite-dimensional H this equivalence no longer holds. Our notion of continuity is equivalent to the usual one in topology. The norm $f \mapsto \|f\|$ is continuous on H, which is tautological given our definition of continuity, because convergence in H has been defined in terms of the norm! I.e., $f_n \to f$ in H *means* $\|f_n - f\| \to 0$, which precisely expresses continuity of the norm. Similarly, according to our definition a bounded operator $a : H \to H$ is clearly continuous, too, for $\|af_n - af\| \to 0$ because $\|af_n - af\| \leq \|a\|\|f_n - f\|$ by (III.5). The main point is that Lemma IV.3 still applies.

Definition IV.4 *A* **compact operator** *on a Hilbert space H is a bounded operator that maps the unit ball $B_1 \subset H$ into a compact set.*

[3] The main theorem below is true in general as well, with a similar proof involving more topology.

[4] Compactness and continuity may be defined for arbitrary topological spaces in this way if one replaces sequences by nets.

This is not the case for any bounded operator, for althoug such operators are continuous, the unit ball in H is not compact.[5] If H is finite-dimensional, so that B_1 *is* compact, then any operator is compact. More generally, a finite-rank operator on an infinite-dimensional Hilbert space (i.e., an operator whose image is finite-dimensional) is compact.

Proposition IV.5 *A bounded operator on a separable Hilbert space is compact iff it is the norm-limit of a sequence of finite-rank operators.*

The proof is left as an exercise, as is the following consequence of the proposition.

Corollary IV.6 *1. If a is compact then so is its adjoint a^*;*

2. If a is compact and b is bounded then ab and ba are compact;

3. A projection p is compact iff it is finite-dimensional.

Using this corollary, it is easy to show that the set of all compact operators in $B(H)$ is a Banach space called $B_0(H)$ in the operator norm. Moreover, $B_0(H)$ is even an algebra under operator multiplication, closed under involution.

Integral operators form an important class of compact operators. Without proof we mention that if $\Omega \subset \mathbb{R}^n$ is compact, any operator of the form $af(x) = \int_\Omega d^n x\, a(x,y) f(y)$ is compact when the kernel $a(-,-)$ is continuous on $\Omega \times \Omega$. More generally, for any $\Omega \subset \mathbb{R}^n$ such an operator is compact when $a(-,-) \in L^2(\Omega \times \Omega)$, i.e., when $\int d^n x d^n y\, |a(x,y)|^2 < \infty$. The following theorem completely characterizes self-adjoint compact operators.

Theorem IV.7 *Let a be a self-adjoint compact operator on a Hilbert space H. Then H has an orthonormal basis (e_i) of eigenvectors of a, in terms of which*

$$a = \sum_i \lambda_i p_i, \tag{IV.2}$$

where p_i projects onto the span of e_i, and the sum converges in the sense that $af = \sum_i \lambda_i p_i f$ for each fixed $f \in H$. Moreover, the set (λ_i) of eigenvalues of a has the property that

$$\lim_{i \to \infty} |\lambda_i| = 0. \tag{IV.3}$$

Conversely, a bounded self-adjoint operator on H of the form (IV.2) where the eigenvalues satisfy (IV.3) is compact.

To prove the first claim, we may simply repeat the proof of Proposition IV.1, as compact operators have been defined for precisely this purpose! In particular, Lemma IV.2 still holds. However, the infinite-dimensional situation makes one big difference: the iteration procedure in the proof is not a priori guaranteed to converge. To settle this, let $p = \sum_i p_i$ (with convergence as understood in (III.18)) be the projection onto the subspace of H spanned by all eigenvectors of a. Clearly, a maps pH onto itself, and using $a^* = a$, it follows that it maps $(pH)^\perp$ onto itself as well: if $g \in (pH)^\perp$ then by definition $(f,g) = 0$ for all $f \in pH$, so $(f, ag) = (a^* f, g) = (af, g) = 0$. But $(pH)^\perp$ is a Hilbert space in its own right, and since the restriction of a to $(pH)^\perp$ is given by $(1-p)a$, this restriction is still compact by Corollary IV.6.2. Hence Lemma IV.2 applies to it, implying that $(1-p)a$ has an eigenvector in $(pH)^\perp$, which is the same as saying that a has an eigenvector in $(pH)^\perp$. This contradicts the definition of pH.

We leave the proof of the second claim as an exercise. ■

Corollary IV.8 *Each eigenvalue of a self-adjoint compact operator except possibly 0 has finite multiplicity, and 0 is the only possibly accumulation point of the set of eigenvalues. Hence we may rewrite (IV.2) as*

$$a = \sum_\alpha \lambda_\alpha p_\alpha, \tag{IV.4}$$

where all eigenvalues λ_α are different and p_α is the finite-dimensional projection $p_\alpha := \sum_{i|\lambda_i = \lambda_\alpha} e_i$.

[5] The unit ball in an infinite-dimensional Hilbert space is not compact in the topology defined by the norm, in which $f_n \to f$ when $\|f_n - f\| \to 0$. Miraculously, the unit ball *is* compact in another topology, namely the so-called weak topology, in which $f_n \to f$ when $|(g, f_n - f)| \to 0$ for each fixed $g \in H$.

This expansion has the advantage over (IV.2) that it is unique; in (IV.2) there is an arbitrariness in the choice of basis within the eigenspace of each eigenvalue with multiplicity greater than one. In particular, the eigenvalues (λ_i) are uniquely determined by a.

Corollary IV.9 *An arbitrary compact operator a on a Hilbert space H has an expansion*

$$af = \sum_i \mu_i (e_i, f) u_i, \tag{IV.5}$$

where (e_i) and (u_i) are orthonormal bases of H, $\mu_i > 0$, and (μ_i^2) are the eigenvalues of a^*a.

Since a^*a is self-adjoint, Theorem IV.7 applies, i.e.,

$$a^*af = \sum_i \lambda_i (e_i, f) e_i. \tag{IV.6}$$

Since a^*a is positive, in the sense that $(f, a^*af) \geq 0$ for all $f \in H$ (for $(f, a^*af) = \|af\|^2$), it follows that $\lambda_i \geq 0$ for each i. Hence $\mu_i = \sqrt{\lambda_i}$ is well defined as the positive square-root. Now define $u_i := \mu_i^{-1} a e_i$. Using (III.18), eq. (IV.5) is immediate. ■

The μ_i are sometimes called the **singular values** of a.

Chapter V

Quantum mechanics and Hilbert space I: states and observables

We are now going to apply the previous machinery to quantum mechanics, referring to the Introduction for history and motivation. The mathematical formalism of quantum mechanics is easier to understand if it is compared with classical mechanics, of which it is a modification. We therefore start with a rapid overview of the latter, emphasizing its mathematical structure.

V.1 Classical mechanics

The formalism of classical mechanics is based on the notion of a **phase space** M and **time-evolution**, going back to Descartes and Newton, and brought into its modern form by Hamilton. The phase space of a given physical system is a collection of points, each of which is interpreted as a possible state of the system. At each instance of time, a given state is supposed to completely characterize the 'state of affairs' of the system, in that:

1. The value of any observable (i.e., any question that may possibly be asked about the system, such as the value of its energy, or angular momentum,...) is determined by it.[1]

2. Together with the equations of motion, the state at $t = 0$ is the only required ingredient for the prediction of the future of the system.[2]

Observables are given by functions f on M. The relationship between states (i.e. points of M) and observables is at follows:

The value of the observable f in the state x is $f(x)$.

This may be reformulated in terms of questions and answers. Here an observable f is identified with the question: *what is the value of f?* A state is then a list of answers to all such questions.

A very basic type of observable is defined by a subset $S \subset M$. This observable is the characteristic function χ_S of S, given by $\chi_S(x) = 1$ when $x \in S$ and $\chi_S(x) = 0$ when $x \notin S$. The corresponding question is: *is the system in some state lying in $S \subset M$?* The answer yes is identified with the value $\chi_S = 1$ and the answer no corresponds to $\chi_S = 0$. Sich a question with only two possible answers is called a **yes-no question**.

In these notes we only look at the special case $M = \mathbb{R}^{2n}$, which describes a physical system consisting of a point particles moving in $\mathbb{R}^n$. We use coordinates $(q, p) := (q^i, p_i)$, where $i = 1, \ldots, n$. The q variable ("position") denotes the position of the particle, whereas the meaning of

[1] Philosophers would say that any quantity pertaining to the system *supervenes* on its states; this means that no change in a given quantity is possibly without a change in the state. For example, most scientists would agree that the mind supervenes on the brain (seen as a physical system).

[2] We do not say that such a prediction is always possible in practice. But *if* it is possible at all, it merely requires the state and the equations of motion.

the p variable ("momentum") depends on the time-evolution of the system. For example, for a free particle of mass m one has the relation $\vec{p} = m\vec{v}$, where v is the velocity of the particle (see below). Let us note that one may look at, say, q^i also as an observable: seen as a function on M, one simply has $q^i(q,p) = q^i$, etc.

Given the phase space M, the specification of the system is completed by specifying a function h on M, called the **Hamiltonian** of the system. For $M = \mathbb{R}^{2n}$ we therefore have h as a function of (q,p), informally written as $h = h(q,p)$. The Hamiltonian plays a dual role:

- Regarded as an observable it gives the value of the energy;
- it determines the time-evolution of the system.

Indeed, given h the time-evolution is determined by **Hamilton's equations**

$$\begin{aligned} \dot{q}^i := \frac{dq^i}{dt} &= \frac{\partial h}{\partial p_i}; \\ \dot{p}_i := \frac{dp_i}{dt} &= -\frac{\partial h}{\partial q^i}. \end{aligned} \tag{V.1}$$

For example, a particle with mass m moving in a potential V has Hamiltonian

$$h(q,p) = \frac{p^2}{2m} + V(q), \tag{V.2}$$

where $p^2 := \sum_{i=1}^n (p_i)^2$. The equations (V.1) then read $\dot{q}^i = p_i/m$ and $\dot{p}_i = -\partial V/\partial q^i$. With the force defined by $F^i := -\partial V/\partial q^i$, these are precisely Newton's equations $d^2q^i/dt^2 = F^i/m$, or $\vec{F} = m\vec{a}$. In principle, h may explicitly depend on time as well.

V.2 Quantum mechanics

Quantum mechanics is based on the postulate that the phase space is a Hilbert space H, with the additional stipulations that:

1. Only vectors of norm 1 correspond to physical states;
2. Vectors differing by a "phase", i.e., by a complex number of modulus 1, correspond to the same physical state.

In other word, $\psi \in H$ and $z\psi$ with $z \in \mathbb{C}$ and $|z| = 1$ give the same state.[3] We here stick to the physicists' convention of denoting elements of Hilbert spaces by Greek letters.[4]

The reason for the first point lies in the probability interpretation of quantum mechanics. The simplest example of this interpretation is given by the quantum mechanics of a particle moving in $\mathbb{R}^3$. In that case the Hilbert space may be taken to be $H = L^2(\mathbb{R}^3)$, and Born and Pauli claimed in 1926 that the meaning of the 'wavefunction' $\psi \in L^2(\mathbb{R}^3)$ was as follows: *the probability* $P(\psi, x \in \Delta)$ *that the particle in state* ψ *is found to be in a region* $\Delta \subseteq \mathbb{R}^3$ *is*

$$P(x \in \Delta|\psi) = (\psi, \chi_\Delta \psi) = \int_\Delta d^3x \, \|\psi(x)\|^2. \tag{V.3}$$

Here χ_Δ is the characteristic function of Δ, given by $\chi_\Delta(x) = 1$ when $x \in \Delta$ and $\chi_\Delta(x) = 0$ when $x \notin \Delta$. It follows that

$$P(x \in \mathbb{R}^n|\psi) = \|\psi\|^2 = (\psi, \psi) = 1, \tag{V.4}$$

[3] It follows that the true state space of a quantum-mechanical system is the **projective** Hilbert space $\mathbb{P}H$, which may be defined as the quotient $SH/\sim$, where $SH := \{f \in H \mid \|f\| = 1\}$ and $f \sim g$ iff $f = zg$ for some $z \in \mathbb{C}$ with $|z| = 1$.

[4] This notation was initially used by Schrödinger in order to make his wave mechanics, a precursor of quantum mechanics, look even more mysterious than it already was.

since by definition of the physical system in question we assume that the particle is somewhere.

More generally, observables are represented in quantum mechanics by self-adjoint operators a on H. In the bounded case ($\|a\| < \infty$) this means $a^* = a$, and the meaning of self-adjointness for unbounded operators will be taken up later. As in classical physics, observables define questions: *what is the value of a?* And once again, a state $\psi \in H$ with $\|\psi\| = 1$ is nothing but a list of answers to such questions. Indeed, the answer to the above question in the state ψ is as follows:

The value of the observable a in the state ψ is $(\psi, a\psi)$.

Although this is a real number, like in classical physics (thanks to $a^* = a$), it now has the interpretation of the **expectation value** of the observable a, rather than its exact value.[5]

In quantum mechanics any projection p defines a so-called yes-no question: *is the system in some state in pH?* Thus projections are the quantum analogues of characteristic functions in classical physics. The fundamental difference between classical and quantum physics, namely the intrinsically statistical character of the latter, is beautifully illustrated by yes-no questions. In the classical case the possible values of χ_S are 0 (no) and 1 (yes). In quantum mechanics the answer to the question p in the state ψ is $(\psi, p\psi)$. If $\psi \in (pH)^\perp$ one has $(\psi, p\psi) = 0$ and if $\psi \in pH$ one has $(\psi, p\psi) = 1$. Indeed, in the former case (no) one can maintain that the state is not in pH, and in the latter case (yes) one can safely say that the state is in pH. In classical physics these are the only possibilities: either $x \in S$ or $x \notin S$. But in quantum mechanics $\psi \in (pH)^\perp$ and $\psi \in pH$ are *not* the only possibilities! In general, one has the decomposition $\psi = \psi^{\|} + \psi^{\perp}$ as explained in Proposition III.6, with both $\psi^{\|}$ and $\psi^{\perp}$ nonzero. Using $p^2 = p^* = p$, one finds

$$(\psi, p\psi) = (\psi^{\|}, p\psi^{\|}) \in [0, 1];$$

the fact that $(\psi, p\psi) \in [0, 1]$ follows from $\|p\| = 1$ from projections (which in turn follows from (III.16)) and (III.5) and Cauchy-Schwarz. Generalizing the interpretation Born and Pauli gave to wavefunctions, we say that:

The number $(\psi, p\psi)$ is the probability that the state ψ lies in pH.

Alternatively:

The probability of the answer yes to the question p in the state ψ is $(\psi, p\psi)$.

V.3 Trace-class operators and mixed states

To be honest, we have only discussed a limited class of states so far, namely the **pure states**. These are states containing maximum information about the system. Hence in classical physics pure states are points in phase space, whereas in quantum mechanics they are unit vectors in Hilbert space. However, in some cases a physics student may not know the precise state of the system, for example because he is drunk. A professor of experimental physics may be in the same situation, this time because he does not know enough theoretical physics to figure out which state he has prepared in the lab. In either case one is unable to distinguish a number of candidate states.

The way out is to make a list of possible pure states (x_k), $x_k \in M$ (in classical physics) or (ψ_k), $\psi_k \in H$ (in quantum physics and assign each state a probability P_k. Of course, one should have $P_k \in [0, 1]$ for each k and $\sum_k P_k = 1$.[6] In classical physics the answer to the question what the value of f is, is then given by

$$\langle f \rangle = \sum_k P_k f(x_k).$$

In quantum physics, the value of a in the given state ρ is

$$\langle a \rangle = \sum_k P_k (\psi_k, a\psi_k). \tag{V.5}$$

[5] What this really means is a matter of ongoing debate. For example, do expectation values refer to outcomes of a long series of measurements? Or to 'propensities' of the observable to have the given expectation value? Or to averages with respect to some unknown theory underlying quantum mechanics? Etcetera

[6] More generally, one take a probability measure μ on M and takes the value of f in the state μ to be $\int_M d\mu\, f$.

In textbooks on quantum mechanics one here introduces a **density matrix**

$$\rho = \sum_k P_k[\psi_k], \tag{V.6}$$

where $[\psi_k]$ is the projection onto the one-dimensional subspace spanned by ψ_k, i.e. (for general unit vectors ψ)

$$[\psi]\varphi := (\psi, \varphi)\psi; \tag{V.7}$$

this is the one-dimensional case of (III.18). Note that physicists write $[\psi] = |\psi\rangle\langle\psi|$ as well as $|\varphi\rangle$ instead of φ; eq. (III.18) then reads

$$|\psi\rangle\langle\psi|\varphi\rangle = |\psi\rangle\langle\psi|\varphi\rangle.$$

This a tautology; it coincides with (III.18) since $\langle\psi|\varphi\rangle = (\psi, \varphi)$. This is one of the few instances where the so-called Dirac notation used in quantum mechanics is actually better than the one in math books.

In any case, one now writes (V.5) as

$$\langle a\rangle = \mathrm{Tr}\,(\rho a). \tag{V.8}$$

Here the **trace** of a (bounded) operator b is defined as follows: take any orthonormal basis (e_i) of H and put

$$\mathrm{Tr}\, b := \sum_i (e_i, be_i). \tag{V.9}$$

This is supposed to be independent of the chosen basis. So if ρ is given by (V.6) and the vectors ψ_k are mutually orthogonal, one may choose a basis that contains all of them. In that case one easily shows that

$$\mathrm{Tr}\,(\rho a) = \sum_k P_k(\psi_k, a\psi_k), \tag{V.10}$$

so that (V.9) and (V.5) are the same.

In quantum mechanics density matrices are often called **mixed states**. If (V.6) contains only one term $\rho = [\psi]$, one has $\mathrm{Tr}\,(\rho a) = (\Psi, a\psi)$ and the state is actually "pure".

We now present the general theory of the trace; this is more complicated than the physics literature suggests. For example, the independence of the trace on the basis chosen is delicate. If $\dim(H) < \infty$ there is no problem; a simple computation shows that

$$\sum_i (e_i, ae_i) = \sum_i (u_i, au_i)$$

for any two o.n.b. (e_i) and (u_i) (just expand u_i in terms of the e_i and interchange summations). However, if $\dim(H) = \infty$ one can find bounded operators $b : H \to H$ and orthonormal bases (u_k) and (e_i) such that $\sum_i (e_i, be_i) = \infty$ and $\sum_k (u_k, be_k) = \infty$ (exercise).

To avoid this, in order to make sense of the trace when H is infinite-dimensional one needs a class of operators a for which (V.9) is i) finite and ii) independent of the basis. This class can be constructed in (at least) two different but equivalent ways. The simplest way is as follows.

1. In order to have a well-defined trace, an operator b needs to be bounded and compact.

2. If b is compact, then so is b^*b (exercise). Morever, b^*b is self-adjoint, since

$$(b^*b)^* = b^*b^{**} = b^*b.$$

3. So we can apply Theorem IV.7 with $a = b^*b$. This yields

$$b^*b = \sum_k \mu_k p_k$$

for certain $\mu_k \in \mathbb{R}$ and projection $p_k : H \to H$. Now, if $\psi \in p_k H$, so that $b^*b\psi = \mu_k\psi$, taking the inner product with ψ one has $(\psi, b^*b\psi) = \mu_k(\psi, \psi)$, i.e. $\|b\psi\|^2 = \mu_k\|\psi\|^2$. Hence $\mu_k \geq 0$.

Definition V.1 *We say that a bounded operator $b : H \to H$ is* **trace-class** *when b is compact and $\sum_k \sqrt{\mu_k} < \infty$. Here the μ_k are the eigenvalues of b^*b. If b is trace-class we write $b \in B_1(H)$.*

Another approach to the trace is based on the notion of the square root of the operator b^*b itself (instead of on the square root of its eigenvalues, as above). Let us call an operator $b : H \to H$ **positive** when $(f, bf) \geq 0$ for all $f \in H$. We write $b \geq 0$. We will often use the simple property that if b is positive, then $b^* = b$. It turns out that *if* b is positive, then (V.9) is independent of the orthonormal basis (e_i); so it is either finite or infinite. If it is finite this defines the trace of b, and we say b is trace-class. This defines the trace for positive operators.

To define the trace in general, one uses the square-root of a positive operator. Namely, one can show (exercise) that if b is positive, then there exists a unique operator $\sqrt{b}$ with the properties $\sqrt{b}^2 = b$ en $\sqrt{b} \geq 0$. In particular, the **absolute value**

$$|b| := \sqrt{b^*b} \tag{V.11}$$

is defined, as we have just seen that b^*b is positive. We now say that an arbitrary bounded operator b is trace-class if $\mathrm{Tr}\,|b| < \infty$, where the trace is given by (V.9). It turns out that b is trace-class in this sense iff it is trace-class according to Definition V.1.

In any case, the most important properties of the trace are:

Theorem V.2 *Suppose b is trace-class, or $b \in B_1(H)$. Then:*

1. *The expression* (V.9)*, called the* **trace of** *b, is absolutely convergent and independent of the orthonormal basis (e_i).*

2. *If a is bounded, then $ab \in B_1(H)$ and $ba \in B_1(H)$ and*

$$\mathrm{Tr}\,(ab) = \mathrm{Tr}\,(ba). \tag{V.12}$$

3. *If u is unitary then*

$$\mathrm{Tr}\,(ubu^{-1}) = \mathrm{Tr}\,(b). \tag{V.13}$$

This theorem is easy to use but by no means easy to prove, so we leave this as a special project. Instead, we return to quantum mechanics.

Definition V.3 *An bounded operator $\rho : H \to H$ is called a* **density operator** *or* **density matrix** *if:*

1. *ρ is positive;*

2. *ρ is trace-class;*

3. $\mathrm{Tr}\,\rho = 1$.

By part 2 of Theorem V.2, for any bounded operator a the expectation value (V.8) is well defined. Furthermore, since ρ is compact (cf. Definition V.1) and self-adjoint (as follows from its positivity), we may apply Theorem IV.7 with $a = \rho$. This yields the expansion (V.6) and we have come full circle.

The above mathematical model of quantum mechanics is too limited, however. The states are OK, but most observables in quantum mechanics turn out to be unbounded. Position and momentum are examples. "It is a fact of life that many of the most important operators which occur in mathematical physics are not bounded" [18]. We now turn to the theory of such unbounded observables.

Chapter VI

Closed unbounded operators

VI.1 The closure

We are now familiar with two classes of operators on a Hilbert space: *bounded* ones, and *compact* ones. As we have seen, the latter are precisely those bounded operators for which a spectral theory analogous to that for matrices exists. It would be possible to develop the spectral theory of general bounded (self-adjoint)operators at this point, but in fact it turns out that this theory can be written down almost without extra effort for the far wider class of *closed* (self-adjoint) operators.

To come to grips with the notion of un unbounded operator, we note the following.

Theorem VI.1 *An operator on a Hilbert space H is bounded iff it is continuous in the sense that $f_n \to f$ implies $af_n \to af$ for all convergent sequences (f_n) in H.*

Let $a : H \to H$ be bounded. By (III.5), if $f_n \to f$ in H, that is, $\|f_n - f\| \to 0$, then $af_n \to af$ in H, since $\|af_n - af\| \leq \|a\|\|f_n - f\|$. Conversely, if a is not bounded, then for each $n \in N$ there is $f_n \in H$ with $\|f_n\| = 1$ and $\|af_n\| \geq n$. The sequence $(g_n = f_n/n)$ converges to 0, but since $\|ag_n\| \geq 1$, the sequence (ag_n) does not converge to $a0 = 0$. Hence a is not continuous, and the implication "continuous $\Rightarrow$ bounded" has been proved by *reductio ad absurdum.* ■

It follows that unbounded operators are discontinuous: if $f_n \to f$ it is not guaranteed that $af_n \to af$; indeed, it is not guaranteed that (af_n) converges at all! Hence an essential difference between the bounded and the unbounded case is that whereas for bounded operators a Proposition III.3 states that even if a is initially defined on some dense subspace D of H, it can uniquely be extended to H by continuity, for unbounded operators a such an extension by continuity will not in general exist. Although a discontinuous extension to H might exist, in practice it is very unusual to talk about unbounded operators a defined on H. This is because interesting unbounded operators tend to be defined on $D \subset H$ by some natural expression, which simply does not make sense on all of H. Consequently, the specification of the subspace D on which a is defined, called the **domain** of a, denoted by $D(a)$ is absolutely essential when a is an unbounded operator.

Recall that a subspace $K \subset H$ is called *dense* in H when for each $f \in H$ there is a sequence (f_n) in K converging to f.

> *Unless explicitly stated otherwise, we always assume that the domain of an operator is dense in H.*

For example, we have seen that $a \in C(\mathbb{R})$ defines a bounded operator on $H = L^2(\mathbb{R})$ by multiplication when $\|f\|_\infty < \infty$, i.e., when a is bounded. When a is unbounded as a function, we cannot really make the natural claim that consequently a is unbounded as a multiplication operator on H, since a does not map H to itself as soon as it is unbounded. What we can say, however, is that a is unbounded as a multiplication operator on the subspace $D(a) = C_c(\mathbb{R})$, which (by our definition of L^2) is dense in H. Other examples are given by differential operators: whereas one cannnot really say that $a = id/dx$ is unbounded on $L^2(\mathbb{R})$ since the derivative of most functions in L^2 is not even defined, one can say that a is unbounded on, say, $D(a) = C_c^1(\mathbb{R}) := C_c(\mathbb{R}) \cap C^1(\mathbb{R})$.

There is some flexibility in the choice of the domain, and the theory of unbounded operators of closable type even largely revolves around the business of enlarging a given domain. Here we define an **extension** of a given operator $a : D(a) \to H$ as an operator $a_1 : D(a_1) \to H$ where $D(a) \subset D(a_1)$ and $a_1 = a$ on $D(a)$; we write $a \subset a_1$. As we have seen, if a is bounded there is only one interesting extension, namely the one defined on any larger domain (including H) by continuity, but in the unbounded case the theory of extension of operators turns out to be very rich indeed. As a rather trivial example, we could have defined $a = id/dx$ initially on $D(a) = C_c^\infty(\mathbb{R}) := C_c(\mathbb{R}) \cap C^\infty(\mathbb{R})$; the same expression $a_1 = id/dx$ but now defined on $D(a_1) = C_c^1(\mathbb{R})$ is formally an extension of a. Similarly, an unbounded mutliplication operator $a \in C(\mathbb{R})$ may initially be defined on $D(a) = C_c^\infty(\mathbb{R})$, to be extended by the same expression defined on $D(a_1) = C_c(\mathbb{R})$, as above. Clearly, the largest possible domain on which a multiplication operator $a \in C(\Omega)$ can be defined in the natural way is

$$D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}. \tag{VI.1}$$

The particular unbounded operators that one can deal with satisfy a relic of continuity. To explain this, we define the **graph** of a as the subset $\{f, af\} \subset H \times H$. To define the notion of closedness in $H \times H$ we equip this set with the structure of a Hilbert space in the following way: we first equip $H \times H$ with the structure of a vector space by defining $\langle f_1, f_2\rangle + \langle g_1, g_2\rangle := \langle f_1 + g_1, f_2 + g_2\rangle$ and $\lambda\langle f_1, f_2\rangle := \langle \lambda f_1, \lambda f_2\rangle$, and subsequently putting an inner product on it by $(\langle f_1, f_2\rangle, \langle g_1, g_2\rangle) := (f_1, g_1) + (f_2, g_2)$. With this structure, $H \times H$ is a Hilbert space called $H \oplus H$, for it is precisely the direct sum of H with itself.

Definition VI.2 *A* **closed operator** $a : D(a) \to H$ *is a linear map from a dense subspace* $D(a) \subset H$ *to* H *for which either of the following equivalent conditions holds:*

- *If* $f_n \to f$ *in* H *for a sequence* (f_n) *in* $D(a)$ *and* (af_n) *converges in* H*, then* $f \in D(a)$ *and* $af_n \to af$ *in* H*.*
- *The graph of* a *is closed.*
- *The domain* $D(a)$ *is closed in the norm* $\|f\|_a^2 := \|f\|^2 + \|af\|^2$*.*

Note that the norm $\|\cdot\|_a$ comes from the new inner product $(f, g)_a := (f, g) + (af, ag)$ on $D(a)$. Hence $D(a)$ is a Hilbert space in the new inner product when a is closed.

It is quite unusual for an operator to be closed in the form initially given. For example, a multiplication operator a in $L^2(\Omega)$ is not closed on $C_c(\Omega)$; in fact, a turns out to be closed only on the domein (VI.1). Fortunately, an operator a that is not closed may often be extended into a closed one. The condition for this to be possible is as follows.

Definition VI.3 *A* **closable operator** $a : D(a) \to H$ *is a linear map from a dense subspace* $D(a) \subset H$ *to* H *with the property that the closure* $G(a)^-$ *of its graph is itself the graph* $G(a^-)$ *of some operator* a^- *(called the* **closure** *of* a*).*

In other words, a^- is a closed extension of a. It is clear that a^- is uniquely defined by its graph $G(a^-) = G(a)^-$.

Proposition VI.4 *An operator* a *is closable iff either of the following equivalent conditions holds:*

- *If* $f_n \to 0$ *for a sequence* (f_n) *in* $D(a)$ *and if* (af_n) *converges, then* (af_n) *must converge to 0.*
- *The closure* $G(a)^-$ *of the graph of* a *does not contain any element of the form* $(0, g)$ *for* $g \neq 0$*.*

In that case, the domain of the closure a^- *of* a *is the set of all* $f \in H$ *to which some sequence* (f_n) *in* $D(a)$ *converges and for which* (af_n) *converges as well. Its action is given by* $a^- f := \lim_n af_n$*.*

Finally, the operator a^- *is the smallest closed extension of* a*.*

To verify that a^- is indeed closed, suppose $f_n \to f$ and $af_n \to g$, with (f_n) in $D(a^-)$. Since $f_n \in D(a^-)$ for fixed n, there exists $(f_{m,n})$ in $D(a)$ such that $\lim_m f_{m,n} = f_n$ and $\lim_m af_{m,n} =: g_n$ exists. Then clearly $\lim_{m,n} f_{m,n} = f$, and we claim that

$$\lim_{m,n} af_{m,n} = g. \tag{VI.2}$$

Namely, $\|af_{m,n} - g\| \leq \|af_{m,n} - af_n\| + \|af_n - g\|$. For $\epsilon > 0$ take n so that the second term is $< \epsilon/2$. For that fixed n, $a(f_{m,n} - f_n)$ converges as $m \to \infty$ because $af_{m,n} \to g_n$ and af_n is independent of m. Also, recall that $f_{m,n} - f_n \to 0$ as $m \to \infty$. By assumption, a is closable, hence by definition one must have $a(f_{m,n} - f_n) \to 0$ in m. Hence we may find m so that $\|af_{m,n} - af_n\| < \epsilon/2$, so that $\|af_{m,n} - g\| < \epsilon$, and (VI.2) follows. Hence $f \in D(a^-)$. Finally, since $a^- f := \lim_{m,n} af_{m,n}$ one has $a^- f = g$ by (VI.2), or $a^- f = \lim_n af_n$ by definition of g. It follows that a^- is closed. This extension of a is clearly the minimal closed one.

This argument shows that for a^- to be closed it is sufficient that a is closable. Conversely, if a fails to be closable it cannot have any closed extension whatsoever, since a^- is by definition linear, and $a^- 0 = 0$ for any operator. The second condition for closability is then clearly equivalent to the first. ■

For example, a multiplication operator a in $H = L^2(\Omega)$ is closable on $C_c(\Omega)$: in both cases the closure has domain (VI.1). On the other hand, an example of a non-closable operator is given by $H = L^2(\Omega)$, $D(a) = C_c(\Omega)$, and $af := f(0)g$, where $g \in H$ is arbitrary.

In general, even closed unbounded operators may have closed extensions, a phenomenon which is particular important in connection with the theory of self-adjointness; see below.

This section would not be complete without mentioning a special case of one of the most famous theorems in functional analysis, namely the **closed graph theorem** (for Hilbert spaces):

Theorem VI.5 *If $a : H \to H$ has a closed graph, then it is bounded. In other words, a closed operator defined on all of H is necessarily bounded.*

We will use this theorem only once, since in applications an operator defined on H is usually already known to be bounded, whereas unbounded operators are never defined on H, so that their graph cannot be studied in any case.[1]

VI.2 Symmetric and self-adjoint operators

The most important closed operators, not just for quantum mechanics also but for mathematics as a whole, are the self-adjoint ones. To define these, first recall the definition of the adjoint a^* in the unbounded case: see Definition III.4.

Although it may even happen that $D(a^*)$ is zero, this is pretty pathological, and in most 'natural' examples $D(a^*)$ turns out to be dense. For example, a multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$, defined on any of the domains we have considered (i.e., $D(a) = C_c^\infty(\Omega)$, $D(a) = C_c(\Omega)$, or (III.17)), has $a^* = \overline{a}$ (i.e., the complex conjugate of a seen as a multiplication operator) defined on $D(a^*)$ given by the right-hand side of (III.17). The following important result shows when $D(a^*)$ is dense.

Proposition VI.6 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

1. *The adjoint a^* is closed.*
2. *The operator a is closable iff $D(a^*)$ is dense.*
3. *In that case, one has $a^- = a^{**}$ and $(a^-)^* = a^*$.*

[1] On the theoretical side, however, an important consequence of the closed graph theorem is another famous result known as the **open mapping theorem**: a bounded surjective operator on a Hilbert space H is open (in that the image of an open set in H is open; the boundedness of H implies the opposite, namely that the inverse image of an open set in H is open).

The proof can be elegantly given in terms of the graph $G(a)$. Defining $U : H \oplus H \to H \oplus H$ by $U(f,g) := (g,-f)$, it is easy to verify that (exercise!)

$$G(a^*) = U(G(a)^\perp) = U(G(a))^\perp. \tag{VI.3}$$

Hence the first claim immediately follows, since any orthogonal complement is closed (cf. Lemma II.10).

By Proposition (II.10) and (VI.3) one has $G(a)^- = G(a)^{\perp\perp} = (U^{-1}G(a^*))^\perp$. But

$$(U^{-1}G(a^*))^\perp = \{\langle f,g\rangle \in H \oplus H \mid (f,a^*h) - (g,h) = 0 \,\forall h \in D(a^*)\}.$$

Consequently, referring to Proposition VI.4, $(0,g) \in G(a)^-$ iff $g \in D(a^*)^\perp$, proving the second claim. Using (VI.3) twice (first for a^*, then for a), we have

$$G(a^{**}) = (UG(a^*))^\perp = (U^2(G(a)^\perp))^\perp = G(a)^{\perp\perp} = G(a)^- = G(a^-),$$

where we have used $U^2 = -1$ and $-G(b) = G(b)$ for any operator b. This proves the first part of the third claim. Finally, if a is closable, then using (VI.3) and Lemma II.10 and (VI.3) once more, we have

$$G(a^*) = U(G(a)^\perp) = U((G(a)^-)^\perp) = U(G(a^-)^\perp) = G((a^-)^*). \qquad \blacksquare$$

We now come to the central definition of this chapter. An equality $a = b$ between unbounded operators always stand for $D(a) = D(b)$ and $a = b$. Similarly, $a \subset b$ means $D(a) \subset D(b)$ and $b = a$ on $D(a)$.

Definition VI.7 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

- *If $a = a^*$, i.e., if $D(a^*) = D(a)$ and $(af,g) = (f,ag)$ for all $f,g \in D(a)$, then a is called* **self-adjoint**.
- *If $a^{**} = a^*$ (equivalently, if a is closable and $a^- = a^*$ or $(a^-)^* = a^*$), then a is called* **essentially self-adjoint**.
- *If $a \subset a^*$ i.e., if $(af,g) = (f,ag)$ for all $f,g \in D(a)$, then a is called* **symmetric**.

It follows Proposition VI.6 that a self-adjoint operator is closed, and that a symmetric operator is closable (because $D(a^*)$, containing $D(a)$, is dense). For a symmetric operator one has $a \subseteq a^- = a^{**} \subseteq a^*$, with equality at the first position when a is closed, and equality at the second position when a is essentially self-adjoint; when both equalities hold, a is self-adjoint. Conversely, an essentially self-adjoint operator is, of course, symmetric. A symmetric operator may or may not have self-adjoint extensions; we will deal with this problem in detail later on. Without proof we quote the **Hellinger–Toeplitz theorem**: *If a is self-adjoint on $D(a) = H$, then a is bounded.* This confirms the idea that it is pointless to try to define unbounded operators on all of H in some manifestly discontinuous way. All this is very subtle, but the following example illustrates at least the easy part of the theory:

Proposition VI.8 *A real-valued multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$ is essentially self-adjoint on $D(a) = C_c^\infty(\Omega)$ and on $D(a) = C_c(\Omega)$, and is self-adjoint on*

$$D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}. \tag{VI.4}$$

Cf. (III.17)). Of course, $D(a) = H$ when $\|a\|_\infty < \infty$, since in that case a is a bounded operator, as we have seen.

The proof is almost trivial: by definition, $D(a^*)$ consists of all $f \in L^2(\Omega)$ for wich the functional $g \mapsto (f,ag) = \int_\Omega d^n x\, \overline{f}(x)a(x)g(x)$ is bounded; for each of the three choices of $D(a)$ listed this implies $\overline{f}a \in L^2(\Omega)$ by Riesz–Fréchet, so that $D(a^*) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}$, with $a^* = \overline{a}$ as a multiplication operator. If a is real-valued, then a^* is self-adjoint by the very same argument, which implies all claims. $\blacksquare$

Chapter VII

Spectral theory for selfadjoint operators

We denote the kernel or null space of a map a by $N(a)$ and its range or image by $R(a)$. As before, $D(a)$ denotes the domain of a. Also, $a - z$ for $z \in \mathbb{C}$ denotes the operator $a - z1$.

VII.1 Resolvent and spectrum

The theory of the spectrum of a closed operator on a Hilbert space (which may be bounded or unbounded) is a generalization of the theory of eigenvalues of a matrix. From linear algebra we recall:

Proposition VII.1 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. The a is injective iff it is surjective.*

This follows from the fundamental fact that if $a : V \to W$ is a lnear map between vector spaces, one has $R(a) \cong V/N(a)$. If $V = W = \mathbb{C}^n$, one one count dimensions to infer that $\dim(R(a)) = n - \dim(N(a))$. Surjectivity of a yields $\dim(R(a)) = n$, hence $\dim(N(a)) = 0$, hence $N(a) = 0$, and vice versa.[1] ■

Corollary VII.2 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. Then $a - z$ is invertible (i.e., injective and surjective) iff z is not an eigenvalue of a, i.e., if there exists no $f \in \mathbb{C}^n$ such that $af = zf$.*

Defining the **spectrum** $\sigma(a)$ of $a : \mathbb{C}^n \to \mathbb{C}^n$ as the set of eigenvalues of a and the **resolvent** $\rho(a)$ as the set of all $z \in \mathbb{C}$ for which $a - z$ is invertible, we therefore have

$$\sigma(a) = \mathbb{C} \backslash \rho(a). \tag{VII.1}$$

If $z \in \rho(a)$, the equation $(a - z)f = g$ for the unknown $f \in \mathbb{C}^n$ has a unique solution for any g; existence follows from the surjectivity of $a - z$, whereas uniqueness follows from its injectivity (if $a - z$ fails to be injective then any element of its kernel can be added to a given solution).

Now, if a is an operator on an infinite-dimensional Hilbert space, it may not have any eigenvalues, even when it is bounded and self-adjoint. For example, if $a(x) = \exp(-x^2)$ the associated multiplication operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is bounded and self-adjoint, but it has no eigenvalues at all: the equation $af = \lambda f$ for eigenvectors is $\exp(-x^2)f(x) = \lambda f(x)$ for (almost) all $x \in \mathbb{R}$, which holds only if f is nonzero at a single point. But in that case $f = 0$ as an element of L^2. However, the situation is not hopeless. More generally, let any $a \in C_b(\mathbb{R})$, interpreted as a multiplication

[1] In general, this proposition yields the very simplest case of the Atiyah–Singer index theorem, for which these authors received the Abel Prize in 2004. We define the **index** of a linear map $a : V \to W$ as $\mathrm{index}(a) := \dim(\ker(a)) - \dim(\mathrm{coker}(a))$, where $\ker(a) = N(a)$ and $\mathrm{coker}(a) := W/R(a)$, provided both quantities are finite. If V and W are finite-dimensional, Proposition VII.1 yields $\mathrm{index}(a) = \dim(V) - \dim(W)$; in particular, if $V = W$ then $\mathrm{index}(a) = 0$ for any linear map a. In general, the index theorem expresses the index of an operator in terms of topological data; in this simple case the only such data are the dimensions of V and W.

operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$. If $x_0 \in \mathbb{R}$ one may find approximate eigenvectors of a in the following sense: take

$$f_n(x) := (n/\pi)^{1/4} e^{-n(x-x_0)^2/2}. \tag{VII.2}$$

Then $\|f_n\| = 1$ and $\lim_{n\to\infty}(a(x) - a(x_0))f_n = 0$, although the sequence f_n itself has no limit in $L^2(\mathbb{R})$. Thus we may call $\lambda = a(x_0)$ something like a generalized eigenvalue of a for any $x_0 \in \mathbb{R}$, and define the spectrum accordingly: let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. We say that $\lambda \in \sigma(a)$ when there exists a sequence (f_n) in $D(a)$ for which $\|f_n\| = 1$ and

$$\lim_{n\to\infty} (a - \lambda)f_n = 0. \tag{VII.3}$$

Of course, when λ is an eigenvalue of a with eigenvector f, we may take $f_n = f$ for all n.

However, this is not the official definition of the spectrum, which is as follows.

Definition VII.3 *Let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. The* **resolvent** *$\rho(a)$ is the set of all $z \in \mathbb{C}$ for which $a - z : D(a) \to H$ is injective and surjective (i.e., invertible). The* **spectrum** *$\sigma(a)$ of a is defined by $\sigma(a) := \mathbb{C}\backslash\rho(a)$.*

Hence the *property* (VII.1) has been turned into a definition! We will prove the equivalence of this definition of the spectrum with the definition above later on. In the example just given, one has $\sigma(a) = a(\mathbb{R})$ if the right domain of a is used, namely (III.17). Thus the spectrum can be nonempty even if there aren't any eigenvalues. The subsequent theory shows that these are precisely the right definitons for spectral theory.

The following result explains the role of closedness.[2]

Proposition VII.4 *If an operator $a : D(a) \to R(a) = H$ has an inverse, then a^{-1} is bounded iff a is closed.*

The proof consists of two steps. First, one has that $a : D(a) \to R(a)$ is closed iff a^{-1} is closed. To prove "$\Rightarrow$", assume $g_n \to g$ and $a^{-1}g_n \to f$. Call $f_n := a^{-1}g_n$; then $af_n = g_n \to g$, so if a is closed then by definition $f \in D(a)$ and $af_n \to af$, so $af = g$, hence $f = a^{-1}g$, which means $a^{-1}g_n \to a^{-1}g$. In particular, $g \in R(a) = D(a^{-1})$, and it follows that a^{-1} is closed. The proof of "$\Leftarrow$" is the same, with a and a^{-1} interchanged. Geometrically, the graph of a^{-1} is just the image of the graph of a in $H \oplus H$ under the map $(f, g) \mapsto (g, f)$, hence if one is closed then so is the other.

Secondly, if $R(a) = H$, then $D(a) = H$, hence a^{-1} is bounded by the closed graph theorem (Theorem VI.5). ∎

Returning to the equation $(a - z)f = g$, it now follows that when $z \in \rho(a)$, the solution f depends continuously on the initial data g iff a is closed. To avoid pathologies, we therefore assume that a is closed in what follows. Furthermore, as we shall see, practically every argument below breaks down when $(a-z)^{-1}$ is unbounded. This also explains why as far as spectral theory is concerned there isn't much difference between bounded operators and closed unbounded operators: in both cases $(a - z)^{-1}$ is bounded for $z \in \rho(a)$.

As an exercise, one easily shows:

Proposition VII.5 *Let a be a closed operator.*

1. *$\rho(a)$ is open (and hence $\sigma(a)$ is closed) in $\mathbb{C}$.*
2. *$\rho(a^*) = \overline{\rho(a)}$; $\sigma(a^*) = \overline{\sigma(a)}$.*

For unbounded operators the spectrum can (literally) be any subset of $\mathbb{C}$, including the empty set.

[2]Some books define the resolvent of a as the set of those $z \in \mathbb{C}$ for which $(a - z)$ is invertible *and* has bounded inverse. In that case, the resolvent is empty when a is not closed.

VII.2 The spectrum of self-adjoint operators

For a general closed operator a, we may decompose the spectrum as

$$\sigma(a) = \sigma_d(a) \cup \sigma_c(a), \tag{VII.4}$$

where the **discrete spectrum** $\sigma_d(a)$ consists of all eigenvalues of a, and the **continuous spectrum** $\sigma_c(a)$ is the remainder of $\sigma(a)$. Recall that eigenvalues lie in $\sigma(a)$, for if $(a-\lambda)f = 0$ for some nonzero f then $a-\lambda$ cannot be injective. The spectrum of self-adjoint operators has a particularly transparent structure.

Theorem VII.6 *Let a be a self-adjoint operator (i.e., $a^* = a$), and let $z \in \mathbb{C}$. Then one of the following possibilities occurs:*

1. *$R(a-z) = H$ iff $z \in \rho(a)$;*
2. *$R(a-z)^- = H$ but $R(a-z) \neq H$ iff $z \in \sigma_c(a)$;*
3. *$R(a-z)^- \neq H$ iff $z \in \sigma_d(a)$.*

The key to the proof is a very simple result.

Lemma VII.7 *If a is closable (equivalently, if $D(a^*)$ is dense), then $R(a-z)^- = N(a^* - \overline{z})^\perp$ and $N(a^* - \overline{z}) = R(a-z)^\perp$.*

Note that the kernel of a closed operator (in this case $a^* - \overline{z}$) is automatically closed. Easy calculations using the definition of a^* yield the inclusions $R(a-z)^\perp \subset N(a^* - \overline{z})$ and $R(a-z) \subset N(a^* - \overline{z})^\perp$. Since $K^{\perp\perp} = K^-$ for any linear subspace K of a Hilbert space, and $K \subset L$ implies $L^\perp \subset K^\perp$, the claim follows. ∎

We first prove Theorem VII.6 for $z \in \mathbb{R}$. If $R(a-z)^- \neq H$, then $N(a-z) = R(a-z)^\perp \neq 0$, so $(a-\lambda)f = 0$ has a nonzero solution and $\lambda \in \sigma_d(a)$. The converse implication has the same proof. If $R(a-z)^- = H$, then $N(a-z) = 0$ and $a-z$ is injective. Now if $R(a-z) = H$ then $a-z$ is surjective as well, and $z \in \rho(a)$. The converse is trivial given the definition of the resolvent. If $R(a-z) \neq H$, then $z \in \sigma_c(a)$ by definition of the continuous spectrum. Conversely, if $z \in \sigma_c(a)$ then $z \notin \sigma_d(a)$ and $z \notin \rho(a)$, so that $R(a-z) = H$ and $R(a-z)^- \neq H$ are exlcuded by the previous 'iff' results for $\rho(a)$ and $\sigma_d(a)$. Hence $R(a-z)^- = H$ but $R(a-z) \neq H$.

To prove Theorem VII.6 for $z \in \mathbb{C}\backslash\mathbb{R}$, we first note that eigenvalues of self-adjoint operators must be real; this is immediate since if $a^* = a$ then $\overline{(f, af)} = (af, f) = (f, af)$, so if f is an eigenvector with eigenvector λ it follows that $\overline{\lambda} = \lambda$. In fact, we will prove that if $z \in \mathbb{C}\backslash\mathbb{R}$, then also $z \in \rho_c(a)$ is impossible, so that $z \in \rho(a)$. To see this we need some lemma's.

Lemma VII.8 *Let a be symmetric. Then $\|(a-z)f\| \geq |\mathrm{Im}\,(z)|\|f\|$.*

Reading Cauchy–Schwarz in the wrong order, we obtain

$$\|(a-z)f\|\|f\| \geq |(f, (a-z)f)| = |(r - i\mathrm{Im}\,(z))\|f\|^2| \geq |\mathrm{Im}\,(z)|\|f\|^2.$$

Here we used the fact that $r := (f, af) - \mathrm{Re}\,(z)$ is a real number by virtue of the symmetry of a. ∎

Hence $z \in \mathbb{C}\backslash\mathbb{R}$ implies $N(a - \overline{z}) = 0$. Combining this with Lemma VII.7, we infer that $R(a-z)^- = N(a-\overline{z})^\perp = H$. To infer that actually $R(a-z) = H$ we need yet another lemma.

Lemma VII.9 *Let a be any densely defined operator. If $\|af\| \geq C\|f\|$ for some $C > 0$ and all $f \in D(a)$, then a is injective and $a^{-1} : R(a) \to D(a)$ is bounded with bound $\|a^{-1}\| \leq C^{-1}$.*

Injectivity is trivial, for $af = 0$ cannot have any nonzero solutions given the bound; a linear map a is injective when $af = 0$ implies $f = 0$. For the second claim, note that

$$\|a^{-1}\| = \sup\{\|a^{-1}g\|, g \in D(a^{-1}) = R(a), \|g\| = 1\} =$$

$$\sup\left\{\left\|a^{-1}\frac{af}{\|af\|}\right\|, f \in D(a), f \neq 0\right\} = \sup\left\{\left\|\frac{f}{\|af\|}\right\|, f \in D(a), f \neq 0\right\}.$$

This yields the claim. ■

Combining this with Lemma VII.8, we see that $z \in \mathbb{C}\backslash\mathbb{R}$ implies $(a-z)^{-1} : D((a-z)^{-1}) \to D(a-z) = D(a)$ is bounded, where $D((a-z)^{-1}) = R(a-z)$. To infer that in fact $R(a-z) = H$, we use:

Lemma VII.10 *If b is closed and injective, then $b^{-1} : R(b) \to D(b)$ is closed.*

See the proof of Proposition VII.4. ■

Lemma VII.11 *If b is closed and bounded, then $D(b)$ is closed.*

This is immediate from the definition of closedness. ■

Taking $b = (a-z)^{-1}$, we find that $D((a-z)^{-1})$ is closed. Since we know that $R(a-z)^- = H$, we conclude that $R(a-z) = H$. The same is true for $\overline{z}$. Hence by Lemma VII.7, $N(a-z) = R(a-\overline{z})^\perp = H^\perp = 0$ and $a - z$ is injective. With $a - z$ already known to be surjective, $z \in \rho(a)$.

The proof of the converse implications is the same as for $z \in \mathbb{R}$, and we have finished the proof of Theorem VII.6. ■

Using similar arguments, one can prove

Theorem VII.12 *Let a be a symmetric operator. Then the following properties are equivalent:*

1. *$a^* = a$, i.e., a is self-adjoint;*
2. *a is closed and $N(a^* \pm i) = 0$;*
3. *$R(a \pm i) = H$;*
4. *$R(a - z) = H$ for all $z \in \mathbb{C}\backslash\mathbb{R}$;*
5. *$\sigma(a) \subset \mathbb{R}$.*

Similarly, the following properties are equivalent:

1. *$a^* = a^{**}$, i.e., a is essentially self-adjoint;*
2. *$N(a^* \pm i) = 0$;*
3. *$R(a \pm i)^- = H$;*
4. *$R(a - z)^- = H$ for all $z \in \mathbb{C}\backslash\mathbb{R}$;*
5. *$\sigma(a^-) \subset \mathbb{R}$.*

The second half of the theorem easily follows from the first, on which we will therefore concentrate. The implications $1 \Rightarrow 2$, $1 \Rightarrow 4$, $1 \Rightarrow 5$ and $2 \Rightarrow 3$ are immediate either from Theorem VII.6 or from its proof. The implications $4 \Rightarrow 3$ and $5 \Rightarrow 4$ are trivial. Thus it only remains to prove $3 \Rightarrow 1$.

To do so, assume $R(a \pm i) = H$. For given $f \in D(a^*)$ there must then be a $g \in H$ such that $(a^* - i)f = (a - i)g$. Since a is symmetric, we have $D(a) \subset D(a^*)$, so $f - g \in D(a^*)$, and $(a^* - i)(f - g) = 0$. But $N(a^* - i) = R(a + i)^\perp$ by Lemma VII.7, so $N(a^* - i) = 0$. Hence $f = g$, and in particular $f \in D(a)$ and hence $D(a^*) \subset D(a)$. Since we already know the opposite inclusion, we have $D(a^*) = D(a)$. Given symmetry, this implies $a^* = a$. ■

Corollary VII.13 *Let $a^* = a$. The $\sigma(a) \subset \mathbb{R}$. In other words, the spectrum of a self-adjoint operator is real.*

As an illustration of Theorem VII.12, one can directly show:

Proposition VII.14 *Let $a \in C(\Omega)$ define a real-valued multiplication operator on*

$$D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\} \subset H = L^2(\Omega),$$

so that $a^* = a$ (cf. Proposition VI.8.) Then the operator a is injective iff $a(x) \neq 0$ for all $x \in \Omega$, and surjective iff there exists $\varepsilon > 0$ so that $|a(x)| \geq \varepsilon$ for all $x \in \Omega$; in that case a is injective and has bounded inverse. Consequently, $\sigma(a) = a(\Omega)^-$, with $a(\Omega) := \{a(x), x \in \Omega\}$.

Finally, we justify our earlier heuristic definition of the spectrum; the thrust of the theorem lies in its characterization of the continuous spectrum, of course.

Theorem VII.15 *Let a be self-adjoint. Then $\lambda \in \sigma(a)$ iff there exists a sequence (f_n) in $D(a)$ with $\|f_n\| = 1$ for all n such that $\lim_n (a - \lambda) f_n = 0$.*

Suppose $\lambda \in \sigma(a)$. If $\lambda \in \sigma_d(a)$ we are ready, taking $f_n = f$ for all n. If $\lambda \in \sigma_c(a)$, then $R(a-\lambda)^- = H$ but $R(a-\lambda) \neq H$ by Theorem VII.6. Now a is self-adjoint, hence a and $a - \lambda$ are closed, so that also $(a-\lambda)^{-1}$ is closed by Lemma VII.10. Hence $(a-\lambda)^{-1} : R(a-\lambda) \to H$ must be a a densely defined unbounded operator by Lemma VII.11, for if it were bounded then its domain would be closed, which $D((a-\lambda)^{-1}) = R(a-\lambda)$ is not, as we have just shown. Thus there is a sequence g_n in $D((a-\lambda)^{-1})$ with norm 1 and $\|(a-\lambda)^{-1} g_n\| \to \infty$. Then $f_n := (a-\lambda)^{-1} g_n / \|(a-\lambda)^{-1} g_n\|$ has the desired property.

Conversely, if $\lambda \in \rho(a)$ then $(a-\lambda)^{-1}$ is bounded, hence $(a-\lambda) f_n \to 0$ implies $f_n \to 0$, so the sequence (f_n) cannot exist, and $\lambda \in \sigma(a)$ by *reductio ad absurdum.* ■

VII.3 Application to quantum mechanics

The theory of self-adjoint operators has many applications, for example to the theory of boundary value problems for linear partial differential equations. In these notes we focus on applications to quantum mechanics.

In Chapter V we initially assumed that observables in quantum mechanics are mathematically represented by bounded self-adjoint operators, i.e. linear maps $a : B(H) \to B(H)$ such that $\|a\| < \infty$ and $a^* = a$. As already mentioned at the end of that chapter, however, this model is too limited. For example, in physics textbooks you will find the position and momentum operators

$$\begin{aligned} \hat{q}^i &= x^i \\ \hat{p}_i &= -i\hbar \frac{\partial}{\partial x^i}. \end{aligned} \tag{VII.5}$$

Here $\hbar \in \mathbb{R}^+$ is a constant of nature, called **Planck's constant**, and $i = 1, 2, 3$. These operators are allegedly defined on $H = L^2(\mathbb{R}^3)$, but we know from the previous chapter that at least $\hat{q}^i$ is unbounded. It is a multiplication operator of the form $a\psi(x) = \hat{a}\psi(x)$ with $\hat{a} \in C(\mathbb{R}^3)$, in this case $\hat{a}(x) = x^i$. As we have seen, a is bounded iff $\|\hat{a}\|_\infty < \infty$, and this clearly not the case for x^i. Hence the position operator is unbounded. It follows from Proposition VI.8 that $\hat{q}^i$ is self-adjoint on the domain

$$D(\hat{q}^i) = \{\psi \in L^2(\mathbb{R}^3) \mid x^i \psi \in L^2(\mathbb{R}^3)\}, \tag{VII.6}$$

where $x^i\psi$ is shorthand for the function $x \mapsto x^i \psi(x)$.

Although we have not had the opportunity to develop the necessary machinery, the story of the momentum operator $\hat{p}_i$ is similar. If we denote the Fourier transform of $\psi \in L^2(\mathbb{R}^3)$ by $\hat{\psi}$, and call its argument $k = (k_1, k_2, k_3) \in \mathbb{R}^3$, we can write

$$\hat{\psi}(k) = \int_{\mathbb{R}^3} d^3x \, \psi(x) e^{-ikx}, \tag{VII.7}$$

where $kx = x^1 k_1 + x^2 k_2 + x^3 k_3$. This inproper integral is defined as follows.

1. Approximate ψ by a sequence (ψ_n) in $C_c(\mathbb{R}^3)$ (i.e. $\lim_{n\to\infty}\psi_n = \psi$ in the norm of $L^2(\mathbb{R}^3)$). This is possible by Proposition II.9.

2. Put
$$\hat{\psi}_n(k) := \int_{\mathbb{R}^3} d^3x\, \psi_n(x) e^{-ikx}, \tag{VII.8}$$
as proper Riemann integrals (the integrand is continuous and since ψ_n has compact support the integral is proper, i.e. over a finite region).

3. It turns out that $(\hat{\psi}_n)$ is a Cauchy sequence in $L^2(\mathbb{R}^3)$, so we may finally define
$$\hat{\psi} := \lim_{n\to\infty} \hat{\psi}_n, \tag{VII.9}$$
where the limit is taken in $L^2(\mathbb{R}^3)$

It turns out that $\psi \in L^2(\mathbb{R}^3)$ iff $\hat{\psi} \in L^2(\mathbb{R}^3)$, and that one can reconstruct ψ from $\hat{\psi}$ by
$$\psi(x) = \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3}\, \hat{\psi}(k) e^{ikx}, \tag{VII.10}$$
which is defined by the same procedure as (VII.7). This reconstruction is as an element of L^2; we cannot recover ψ as an element of $\mathcal{L}^2$ from its Fourier transform. Thus (VII.10) holds "almost everywhere" but not for all x.

The correct domain of the momentum operator $\hat{p}_i$ is then as follows:
$$D(\hat{p}_i) = \{\psi \in L^2(\mathbb{R}^3) \mid k_i\hat{\psi} \in L^2(\mathbb{R}^3)\}. \tag{VII.11}$$
On this domain one has $\hat{p}_i^* = \hat{p}_i$, i.e. the momentum operator is self-adjoint.

In general, any quantum-mechanical observable a should be a self-adjoint operator on some Hilbert space. Bu Corollary VII.13, this implies that the spectrum of a is real, and we will see later that the spectral theorem for self-adjoint operators enables one to construct yes-no questions similar to χ_Δ for the position operator (see (V.3) and surrounding text).

VII.4 The Hamiltonian

In case that the observable is the Hamiltonian, more detailed statements can be made, as follows.

Hamilton's equations of motion for classical mechanics were given in (V.1) and (V.2). Quantum mechanics has a single equation of motion, known as the **Schrödinger equation**. The role of the classical Hamiltonian $h = h(p, q)$ (i.e. a function on phase space) is now played by a certain operator h on a Hilbert space H, whose specification is part of the definition of a given physical system. The precise form of this operator is usually guessed from the form of the classical Hamiltonian. For example, if $H = L^2(\mathbb{R}^3)$ and the classical Hamiltonian is (V.2), Schrödinger took the quantum Hamiltonian to be
$$h = -\frac{\hbar^2}{2m}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} + V. \tag{VII.12}$$

Here m is the mass of a particle moving in a potential V, seen as a a multiplication operator. For example, if the particle is an electron in a hydrogen atom, the potential is given by $V(x) = -e/|x|$.

It is clear that h cannot be defined on all of $L^2(\mathbb{R}^3)$: the partial derivatives of an arbitrary $\psi \in L^2(\mathbb{R}^3)$ will not be defined (and even if they are defined the result may not be square-integrable), and the product $V\psi$ may not lie in $L^2(\mathbb{R}^3)$ either, especially when the potential is singular (as is the case for the hydrogen atom and many other examples).

Hence h is an unbounded operator, and we have to find a domain on which it is self-adjoint. Even for $V = 0$ this is a nontrivial problem. The solution is similar to the case of the momentum operator: it turns out that the free Hamiltonian
$$h_0 = -\frac{\hbar^2}{2m}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} \tag{VII.13}$$

is self-adjoint on the domain

$$D(h_0) = \{\psi \in L^2(\mathbb{R}^3) \mid k^2\hat{\psi} \in L^2(\mathbb{R}^3)\}, \tag{VII.14}$$

with $k^2 = k_1^2 + k_2^2 + k_3^2$. For nonzero potential the problem is very difficult, although most realistic cases have been completely understood now [5, 8, 19, 20, 21, 24, 27]. All known examples support the following interpretation of the spectrum of the Hamiltonian:

- The discrete spectrum $\sigma_d(h)$ corresponds to the bound states of the system;
- The continuous spectrum $\sigma_c(h)$ corresponds to the scattering states.

To clarify this, first note that if $E \in \sigma_d(h)$, by definition there is an eigenvector ψ_E such that $h\psi_E = E\psi_E$. Hence ψ_E is a solution to the time-independent Schrödinger equation with energy E. For example, for the hydrogen atom one has $E_n = -m_e e^4/2\hbar^2 n^2$, where m_e is the mass of the electron and e is its charge, with the well-known eigenfunctions $\psi_{(n,l,m)}$. Such an eigenfunction describes a bound state, in which the electron forms a standing wave around the nucleus.

There is an interesting difference between the classical and the quantum-mechanical description of bound states: a planet revolving around the sun is in a bound state, but it clearly displays time-dependent behaviour (it moves around)! An electron in a bound state, on the other hand, evolves according to the time-dependent Schrödinger equation. We will turn to the precise mathematical meaning of this equation in the next section, but for the moment we just write it down:

$$h\psi(t) = i\hbar\frac{d\psi(t)}{dt}. \tag{VII.15}$$

This equation should be seen as the quantum-mechanical analogue of Hamilton's equations (V.1). If $E \in \sigma_d(h)$, a possible solution of (VII.15) is

$$\psi_E(t) = e^{-itE/\hbar}\psi_E. \tag{VII.16}$$

Although formally $\psi_E(t)$ changes in time, physically nothing really happens, as $\psi_E(s)$ and $\psi_E(t)$ for $s \neq t$ merely differ by a phase factor. Hence any expectation value $(\psi_E(t), a\psi_E(t))$ is independent of t. So bound states in quantum mechanics are static, whereas in classical mechanics they are dynamical. This makes the transition from quantum mechanics to classical mechanics in the limit $\hbar \to 0$ very difficult.

In any case, given $h = h^*$ we may split up the Hilbert space H on which h acts by $H = H_d \oplus H_c$, where H_d contains all eigenvectors of h ans $H_c = H_d^{\perp}$. States in H_c *really* move in time, and physically turn out to describe situations in which a particle moves in space in a nonclosed trajectory. For example, think of a comet moving into the solar system with such a speed that it is not captured by the gravitational pull of the sun, but moves out again. In atomic physics, think of an electron shot into an atom and, after being scattered, moving out again.

VII.5 Stone's theorem

The time-dependent Schrödinger equation (VII.15) is very delicate, mathematically speaking. Let us start with the left-hand side. The Hamiltonian h is generally an unbounded operator, so we should worry about its domain and possible self-adjointness (in order to qualify as an observable). The right-hand side involves a limit, since by definition

$$\frac{d\psi(t)}{dt} := \lim_{s\to 0}\frac{\psi(t+s) - \psi(t)}{s}. \tag{VII.17}$$

Since for fixed t the object $\psi(t)$ is an element of a Hilbert space H, the natural meaning of this limit is to take it in the natural norm of H (i.e., as always, the one derived from the inner product). The *existence* of the limit then means: for each fixed t there is a vector $\dot{\psi}(t) \in H$ such that

$$\lim_{s\to 0}\left\|\frac{\psi(t+s) - \psi(t)}{s} - \dot{\psi}(t)\right\| = 0. \tag{VII.18}$$

If it exists, the vector $\dot{\psi}(t)$ is by definition the time-derivative $d\psi(t)/dt$ (as the notation already suggests). But why should this limit exist?

Hence both the left-hand side and the right-hand side of the time-dependent Schrödinger equation (VII.15) are problematic. **Stone's Theorem** provides a complete mathematical meaning of the time-dependent Schrödinger equation and in fact relates the problem on one side to that on the other. In doing so, it provides an explanation of self-adjointness as well. Stone's Theorem is generally regarded as a highlight in the interaction between Hilbert space theory and quantum mechanics (although it may be considered a theorem in pure mathematics if so desired).

Stone's theorem can be read in two directions:

1. Given the Hamiltonian h as a self-adjoint operator, it defines the time-evolution $\psi(t)$.

2. Given the time-evolution $\psi(t)$, it defines the Hamiltonian h as a self-adjoint operator.

Thus the theorem provides a relationship between the global time-evolution and the 'infinitesimal' time-evolution given by the Hamiltonian and the Schrödinger equation.

We already know what a self-adjoint operator is. To state the theorem, we need to define the notion of time-evolution on a Hilbert space. We motivate this definition by some intuition from quantum mechanics. Physicists solve the time-dependent Schrödinger equation with initial value $\psi(0) = \psi$ by

$$\psi(t) = u(t)\psi, \tag{VII.19}$$

where

$$u(t) = e^{-ith/\hbar}. \tag{VII.20}$$

Here we assume that the Hamiltonian h is time-independent. Indeed, if h is bounded (a situation that rarely occurs in practice except when H is finite-dimensional) the exponential in (VII.20) can simply be defined by a norm-convergent power-series (exercise!). When h is not bounded the exponential *cannot* be defined in this way. We will define the exponential of an unbounded operator in the next chapter using spectral calculus.

Some desirable properties of $u(t)$ may be read off nonetheless from "Australian style" formal computation with the motto *no worries* about any mathematical problem that might arise. We then take these heuristic properties as axioms.

First, we expect that $(\psi(s))(t) = \psi(s+t)$, and this indeed follows from (VII.20) and the formal computation $\exp(ta)\exp(sa) = \exp((s+t)a)$, where a is any operator. Indeed, this is rigorously true when a is bounded. This translates into the property

$$u(s)u(t) = u(s+t) \tag{VII.21}$$

for all $s, t \in \mathbb{R}$. Furthermore, one clearly has

$$u(0) = 0 \tag{VII.22}$$

and the strong continuity property

$$\lim_{t\to 0} u(t)\psi = \psi \tag{VII.23}$$

for each $\psi \in H$. for each $s \in \mathbb{R}$. Finally, each $u(t)$ is unitary.[3] This follows from (VII.20) by a formal computation:

$$u(t)u(t)^* = e^{-ith/\hbar}(e^{-ith/\hbar})^* = e^{-ith/\hbar}e^{ith^*/\hbar} = e^{-ith/\hbar}e^{ith/\hbar} = 1,$$

and similarly for $u(t)^*u(t) = 1$. Here we have used $h^* = h$.

To some up, intuition based on the Schrödinger equation suggests the following idea.[4]

[3] Recall that an operator u is unitary when $uu^* = u^*u = 1$.

[4] Those familiar with groups and representations will recognize that this is just the definition of a continuous unitary representation of $\mathbb{R}$ as a topological group. Condition (VII.23) can be shown to be equivalent to the continuity of the map $\langle t, \psi\rangle \mapsto u(t)\psi$ from $\mathbb{R} \times H$ to H.

Definition VII.16 *A time-evolution on H is a map $\mathbb{R} \to B(H)$, $t \mapsto u(t)$, with the properties (VII.21), (VII.22) and (VII.23) and where $u(t)$ is unitary for each t.*

We now state Stone's theorem. We put $\hbar = 1$ for simplicity (put it back as an exercise!).

Theorem VII.17 *1. Let $t \mapsto u(t)$ be a time-evolution on H. Define an operator h by the domain*

$$D(h) : \{\psi \in H \mid \lim_{s\to 0} \frac{u(s)-1}{s}\psi \text{ exists}\} \tag{VII.24}$$

and the action

$$h\psi := i \lim_{s\to 0} \frac{u(s)-1}{s}\psi. \tag{VII.25}$$

Then $D(h)$ is dense in H and h is self-adjoint.

2. Provided $\psi \in D(h)$, for each $t \in \mathbb{R}$ the vector $\psi(t) = u(t)\psi$ lies in $D(h)$ and satisfies the time-dependent Schrödinger equation

$$h\psi(t) = i\frac{d\psi(t)}{dt}. \tag{VII.26}$$

3. Given a (densely defined) self-adjoint operator h on H there exists a unique time-evolution on H that is related to h in the way just specified. Explicitly, one has

$$u(t) = e^{-ith}, \tag{VII.27}$$

where the exponential function is defined by the spectral calculus.

The last sentence will be explained and proved in the next chapter.

We now prove part 1. Part 2 is an exercise in proving the interchange of limits

$$\lim_{s\to 0} \frac{u(t+s)\psi - u(t)\psi}{s} = u(t) \lim_{s\to 0} \frac{\psi(s)-\psi}{s}. \tag{VII.28}$$

Part 3 will be proved in the next chapter. The proof of part 1 is based on the following lemma.

Lemma VII.18 *Suppose h is a symmetric operator, i.e. $D(h)$ is dense and*

$$(h\varphi, \psi) = (\varphi, h\psi) \tag{VII.29}$$

for all $\varphi, \psi \in D(h)$. If $R(h+i) = H$ and $R(h-i) = H$, then h is self-adjoint.

This is contained in Theorem VII.12. In that theorem, as in all preceding material, it is assumed that $D(h)$ is dense in H. We prove this as follows (leaving the details as an exercise).

For any $\psi \in H$ and $n \in \mathbb{N}$ define

$$\psi_n := n \int_0^\infty ds\, e^{-ns} u(s)\psi. \tag{VII.30}$$

Then $\psi_n \in D(h)$ and $\psi_n \to \psi$. Hence $D(h)$ is dense in H.

The property (VII.29) is an easy application of the definition of h in the statement of Theorem VII.17 and of Definition VII.16 (exercise).

Finally, one shows that $R(h-i) = H$ using a trick: compute that $(h-i)\psi_1 = -i\psi$, with ψ_1 defined by (VII.30) with $n = 1$. The property $R(h-i) = H$ is proved in a similar way.

We have now checked the conditions of Lemma VII.18 and we are finished! ■

So far, we have thought of $t \mapsto u(t)\psi$ as the time-evolution of ψ. But nothing has relied on this interpretation (this is the power of abstraction in mathematics!). Consider the following example. Take $H = L^2(\mathbb{R})$ and define the map $t \mapsto u(t)$ by

$$(u(t)\psi)(x) := \psi(x-t). \tag{VII.31}$$

It is an exercise to show that the map $t \mapsto u(t)\psi$ satisfies Definition VII.16. Using superior foresight, we now rename the operator h defined in Part 1 of Theorem VII.17 as $\hat{p}$. Then (VII.24) is just

$$D(\hat{p}) := \{\psi \in L^2(\mathbb{R}) \mid \psi' \in L^2(\mathbb{R})\}, \tag{VII.32}$$

where the derivative ψ' is defined as follows:

$$\psi'(x) := \lim_{s\to 0} \frac{\psi(x+s) - \psi(x)}{s} \tag{VII.33}$$

the limit not being meant pointwise in x but in the norm of $L^2(\mathbb{R})$. Reinserting $\hbar$, the action (VII.25) of $\hat{p}$ is

$$\hat{p}\psi = -i\hbar \frac{d\psi}{dx}. \tag{VII.34}$$

This is indeed the usual momentum operator, and Stone's theorem states that it is self-adjoint on the domain (VII.32). The theory of the Fourier transform finally shows that the domains (VII.32) and (VII.11) coincide.

More generally, the domains of many operators of interest in quantum theory can be determined through Stone's theorem.

Chapter VIII

The spectral theorem

In this chapter we prove the spectral theorem for self-adjoint operators a. This theorem generalizes the expansion or spectral decomposition (see Theorem IV.7)

$$a = \sum_i \lambda_i p_i \tag{VIII.1}$$

of a self-adjoint compact operator (such as a hermitian matrix) in terms of its eigenvalues λ_i and the projections p_i of the corresponding eigenspaces (i.e., if $\psi \in p_i H$ then $a\psi = \lambda_i \psi$). Let us note the properties

$$p_i \perp p_i \quad (i \neq j) \tag{VIII.2}$$

(since the eigenvectors belonging to different eigenvalues are orthogonal) and

$$\sum_i p_i = 1 \tag{VIII.3}$$

(for the eigenvectors form an orthonormal basis).

This spectral decomposition plays a leading role in the probability interpretation of quantum mechanics, which reads as follows *in case the observable $a = a^*$ is a compact operator*:

1. The possible values of the observable $a : H \to H$ that may be found when it is measured are its eigenvalues $\lambda_i \in \mathbb{R}$;

2. The probability that λ_i occurs when a is measured when the system is in a state $\psi \in H$ (i.e. a unit vector) is
$$P(a = \lambda_i|\psi) = (\psi, p_i\psi) = \|p_i\psi\|^2. \tag{VIII.4}$$

Here we have used the standard notation for conditional probabilities. In particular, when p_i is one-dimensional and $e_i \in p_i H$ is a unit vector one has the Born rule

$$P(a = \lambda_i|\psi) = |(e_i, \psi)|^2. \tag{VIII.5}$$

As we have pointed out before, in general a self-adjoint operator need not have any eigenvalues at all (recall the example of the multiplication operator $a(x) = \exp(-x^2)$ on $H = L^2(\mathbb{R})$), or may have mixed spectrum consisting of both eigenvalues and continuous spectrum (for example, a multiplication operator $a \in C(\Omega)$ on $L^2(\Omega)$ with compact support has eigenvalue 0 with infinite multiplicity, since any ψ with support disjoint from a satisfies $a\psi = 0$, whereas the remainder of the range of a will form its continuous spectrum).

Hence, given $a = a^*$, we need to generalize:

- The map $\lambda_i \mapsto p_i \equiv p(\{\lambda_i\})$ from the spectrum of a to the set of projections on H;
- The expansion (VIII.1).

VIII.1 Spectral measures

We start with the former. The appropriate generalization turns out to be a map $B \mapsto p(B)$ from the Borel subsets[1] of $\mathbb{R}$ to the set of projections on H. This map, called the **spectral measure** on $\mathbb{R}$ defined by a, will have the following properties.

Definition VIII.1 *A map $B \mapsto p(B)$ from the Borel subsets of $\mathbb{R}$ to the set of projections on H is called a* **spectral measure** *when:*

1. $p(\emptyset) = 0$;
2. $p(\mathbb{R}) = 1$;
3. $p(A \cap B) = p(A)p(B)$;
4. $p(A \cup B) = p(A) + p(B)$ *when* $A \cap B = \emptyset$;
5. $p(\cup_n B_n) = \vee p(B_n)$, *where* $\vee p_n$ *is the smallest projection* p *such that* $p_n \leq p$ *for all* n.

Note that 1. follows from 4. It follows from the third item that all $p(B)$ commute among each other when B varies, since $A \cap B = B \cap A$. It also follows that

$$p(A)p(B) = 0 \text{ if } A \cap B = \emptyset. \tag{VIII.6}$$

It will also turn out that $p(B) = 0$ if $B \cap \sigma(a) = \emptyset$ (see Cor. VIII.10), so that the spectral measure of a may be regarded as a map from the Borel sets in $\sigma(a)$ to the set of projections on H. This property allows us to write down the map $B \mapsto p(B)$ for compact self-adjoint operators: if a is compact and $a^* = a$ one has

$$p(B) = \sum_{i|\lambda_i \in B} p_i. \tag{VIII.7}$$

In particular, $p_i = p(\{\lambda_i\})$ as already mentioned. The property (VIII.2) is then a special case of (VIII.6), and (VIII.3) follows from properties 2, 4 and 5 in Definition VIII.1.

Given a self-adjoint operator a, we will construct a spectral measure $B \mapsto p(B)$ by means of

$$p(B) = \chi_B(a). \tag{VIII.8}$$

Here $\chi_B : \mathbb{R} \to \{0, 1\}$ is the characteristic function of B, but we will show how to define it with a self-adjoint operator instead of a real number as its argument. In terms of this spectral measure associated to a, the probability interpretation of quantum mechanics *for arbitrary self-adjoint operators* is as follows:

1. The possible values of $a : D(a) \to H$ that may be found when it is measured are the elements of its spectrum $\sigma(a)$;
2. The probability that some value within $B \subset \sigma(a)$ occurs when a is measured when the system is in a state $\psi \in H$ is
$$P(a \in B|\psi) = (\psi, p(B)\psi) = \|p(B)\psi\|^2. \tag{VIII.9}$$

For example, take the position operator $\hat{q}$ on $L^2(\mathbb{R})$ with domain

$$D(\hat{q}) = \{\psi \in L^2(\mathbb{R}) \mid x\psi \in L^2(\mathbb{R})\} \tag{VIII.10}$$

and action $\hat{q}\psi(x) = x\psi(x)$; see (VII.5) and (VII.6). This operator is self-adjoint; see Proposition VI.8. It turns out that

$$p(B) = \chi_B \tag{VIII.11}$$

[1] If you are unfamiliar with this concept, think of just any "reasonable' subset of $\mathbb{R}$. For example, all open subsets of $\mathbb{R}$ as well as all countable intersections of open sets are Borel, as are all closed subsets of $\mathbb{R}$ and all countable unions thereof. In fact, it is practically (though not logically) impossible to construct a subset of $\mathbb{R}$ that is not Borel!

as a multiplication operator on $L^2(\mathbb{R})$. Hence (VIII.9) becomes

$$P(\hat{q} \in B|\psi) = \int_{\mathbb{R}} dx\, \chi_B(x)|\psi(x)|^2 = \int_B dx\, |\psi(x))|^2. \tag{VIII.12}$$

See also (V.3). More generally, the multiplication operator a on $L^2(\Omega)$ defined by $\hat{a} \in C(\Omega)$ (i.e. $a\psi = \hat{a}\psi$) gives rise to the spectral measure

$$p(B) = \chi_{\hat{a}^{-1}(B)}, \tag{VIII.13}$$

where $\hat{a}^{-1}(B) = \{x \in \Omega \mid \hat{a}(x) \in B\}$. Hence

$$P(a \in B|\psi) = \int_{\hat{a}^{-1}(B)} d^n x\, |\psi(x)|^2. \tag{VIII.14}$$

A completely different example is provided by the unit operator $a = 1 = \mathrm{id}$, which leads to

$$p(B) = 1 \text{ if } 1 \in B; \tag{VIII.15}$$
$$p(B) = 0 \text{ if } 1 \notin B. \tag{VIII.16}$$

Hence

$$P(\mathrm{id} \in B|\psi) = 1 \text{ if } 1 \in B; \tag{VIII.17}$$
$$P(\mathrm{id} \in B|\psi) = 0 \text{ if } 1 \notin B. \tag{VIII.18}$$

In other words, the unit operator assumes the value 1 with probability one.

More generally, suppose $\sigma(a)$ is discrete. In that case the spectral theorem below will take the same form (VIII.1) as for compact operators. One then recovers (VIII.7), so that

$$P(a \in B|\psi) = \sum_{i|\lambda_i \in B} (\psi, p_i\psi). \tag{VIII.19}$$

Let us write

$$P_\psi(B) := (\psi, p(B)\psi), \tag{VIII.20}$$

for the probabilities defined by a given spectral measure on H and a unit vector $\psi \in H$; if the spectral measure is derived from a self-adjoint operator a one of course has $P_\psi(B) = P(a \in B|\psi)$ as in (VIII.9). It now follows from Definition VIII.1 and $\|\psi\| = 1$ that the numbers $P_\psi(B)$ define a probability measure on $\mathbb{R}$ in the following sense.

Definition VIII.2 *A map $B \mapsto P(B)$ from the Borel subsets of $\mathbb{R}$ to $[0,1]$ is called a* **probability measure** *when:*

1. $P(\mathbb{R}) = 1$;
2. $P(\cup_n B_n) = \sum_n P(B_n)$ *whenever* $B_i \cap B_j = \emptyset$ *for* $i \neq j$.

Note that $P(A \cup B) = P(A) + P(B)$ when $A \cap B = \emptyset$ is a special case of the second property, from which $P(\emptyset) = 0$ follows by taking $A = \emptyset$.

This shows that a quantum-mechanical observable (i.e. a self-adjoint operator) a and a state (i.e. a unit vector) ψ in a Hilbert space H together define a probability measure on $\mathbb{R}$ through (VIII.8) and (VIII.20). This should be compared with the "classical" situation, in which one starts with a measure space X, a probability measure[2] μ on X, and a measurable function $f : X \to \mathbb{R}$. From these data, one obtains a probability measure P on $\mathbb{R}$ by $P(B) := \mu(f^{-1}(B))$. Clearly, X, μ and f play the roles of H, ψ and a, respectively. Here $\mathbb{R}$ may be replaced by $f(X) \subset \mathbb{R}$, just as $\mathbb{R}$ may be replaced by $\sigma(a) \in \mathbb{R}$ in the Hilbert space situation.

[2]This is a map from the measurable subsets $\Sigma \subset X$ to $[0,1]$ satisfying $\mu(X) = 1$ and $\mu(\cup_n \Sigma_n) = \sum_n \mu(\Sigma_n)$ whenever $\Sigma_i \cap \Sigma_j = \emptyset$ for $i \neq j$. Just think of $X = \mathbb{R}^n$ and a continuous function $\rho : \mathbb{R}^n \to \mathbb{R}^+$ such that $\int_{\mathbb{R}^n} d^n x\, \rho(x) = 1$. Then $\mu(\Sigma) = \int_\Sigma d^n x\, \rho(x)$.

VIII.2 Construction of spectral measures

Now that we know the goal, we are going to make sense of (VIII.8). We do this for bounded self-adjoint operators a; the unbounded case will be dealt with later. The idea is this. For a polynomial $p(x) = \sum_{k=1}^n c_k x^k$ on $\mathbb{R}$, it is clear what $p(a)$ should mean, namely $p(a) = \sum_{k=1}^n c_k a^k$. We now approximate χ_B by polynomials $(p)_n$ pointwise, $p_n(x) \to \chi_B(x)$ for all $x \in \mathbb{R}$ (see below for a caveat and a precise version). We then define $\chi_B(a)$ and hence $p(B)$ by $\lim_n p_n(a)$, where the limit has to be taken in a certain way (see below). This procedure is justified by the following lemma's.

Lemma VIII.3 *Let $K = [-k, k] \subset \mathbb{R}$, $k \in \mathbb{R}^+$. For each positive bounded (Borel) function $f : K \to \mathbb{R}$ there exists a bounded monotone increasing sequence (p_n) of polynomials on K that converges pointwise to f.*

This means that

$$0 \leq p_0(x) \leq p_1(x) \leq \cdots p_n(x) \leq p_{n+1}(x) \leq \cdots \leq c$$

for some $c > 0$ and all $x \in K$, and

$$\lim_{n\to\infty} p_n(x) = f(x) \tag{VIII.21}$$

for all $x \in K$. We will not prove this lemma from real analysis, as it has nothing to do with Hilbert space theory.

Lemma VIII.4 *1. If p is a real polynomial on K and $p(x) \geq 0$ for all $x \in K$, then $p(a) \geq 0$.*

2. Consequently, if (p_n) is a monotone increasing sequence (p_n) of real polynomials on K bounded by c, then the sequence of operators $(a_n := p_n(a))$ satisfies

$$0 \leq p_0(a) \leq p(a)_1 \leq \cdots p_n(a) \leq p_{n+1}(a) \leq \cdots \leq c1. \tag{VIII.22}$$

Recall that $a \leq b$ for two bounded operators means that $(\psi, a\psi) \leq (\psi, b\psi)$ for all $\psi \in H$. The second part clearly follows from the first part. The proof of this first part is based on another lemma, which is of independent interest:

Lemma VIII.5 *If pq is the pointwise product of two (possibly complex-valued) polynomials p and q, then $(pq)(a) = p(a)q(a)$, and similarly for $p + q$ and cp, $c \in \mathbb{R}$. Moreover, one has $p(a)^* = \overline{p}(a)$ (where $\overline{p}$ is the complex conjugate of p).*

The proof is a simple calculation (exercise). We now derive part 1 of Lemma VIII.4 from Lemma VIII.5. Since $p(x) \geq 0$ for all $x \in K = [-k, k]$, we may write p as

$$p(x) = c \prod_i (x - r_i) \prod_j (s_j - x) \prod_k ((x - t_k)^2 + c_k), \tag{VIII.23}$$

with $c \geq 0$, $c_k \geq 0$, $r_i < -k$ and $s_j > k$. By Lemma VIII.4 we have

$$p(a) = c \prod_i (a - r_i) \prod_j (s_j - a) \prod_k ((a - t_k)^2 + c_k). \tag{VIII.24}$$

It follows from the definition of the operator norm that if $a^* = a$ and $r < -\|a\|$, then $a - r \geq 0$. Similarly, if $s > \|a\|$, then $s - a \geq 0$. Third, if $t \in \mathbb{R}$ then $(a - t)^2 \geq 0$. Finally, if operators b_k all commute and $b_k \geq 0$ for all k, then $\prod_k b_k \geq 0$. This shows that $p(a) \geq 0$. ∎

We say that a sequence (a_n) of bounded self-adjoint operators is monotone increasing bounded when

$$a_0 \leq a_1 \leq \cdots a_n \leq a_{n+1} \leq \cdots \leq c1 \tag{VIII.25}$$

for some constant c.

Lemma VIII.6 *Each monotone increasing bounded sequence (a_n) of bounded self-adjoint operators converges strongly to a bounded self-adjoint operator. This means that for any fixed $\psi \in H$ one has*

$$\lim_n a_n\psi = a\psi \tag{VIII.26}$$

for some bounded self-adjoint operator a. We write this as

$$a = s\text{-}\lim_n a_n. \tag{VIII.27}$$

The proof relies on a generalized Cauchy–Schwartz inequality: if $a \geq 0$, then

$$|(\varphi, a\psi)|^2 \leq (\psi, a\psi)(\varphi, a\varphi) \tag{VIII.28}$$

for all $\psi, \varphi \in H$. The proof is an exercise. Using this inequality, one easily shows that $(a_n\psi)$ is a Cauchy sequence in H. We call its limit $a\psi$, and this defines (VIII.26). Then a is bounded. For we have $\|a\psi\| \leq \|(a - a_n)\psi\| + \|a_n\psi\|$; the first term is as small as you like for large n, whereas $\|a_n\psi\| \leq c\|\psi\|$ because $a_n \leq c1$. Hence $\|a\psi\| \leq c\|\psi\|$ for all $\epsilon > 0$. Self-adjointness is easy as well: $a\psi = \lim_n a_n\psi$ and $a_n^* = a^n$ for all n imply

$$(\varphi, a\psi) = \lim_n (\varphi, a_n\psi) = \lim_n (a_n\varphi, \psi) = (a\varphi, \psi). \qquad \blacksquare$$

Now take K such that $[-\|a\|, \|a\|] \subset K$ (see below why) and use Lemma VIII.3 to find a bounded monotone increasing sequence (p_n) of polynomials on K that converges pointwise to a given positive bounded Borel funtion f. We then put

$$f(a) := \text{s-}\lim p_n(a), \text{ where } p_n(x) \to f(x)\, \forall x \in K. \tag{VIII.29}$$

This is independent of the approximating sequence (p_n).

We are now in a position to make sense of (VIII.8) for a bounded and self-adjoint; just take $f = \chi_B$ in (VIII.29) to define

$$\chi_B(a) := \text{s-}\lim p_n(a), \text{ where } p_n(x) \to \chi_B(x)\, \forall x \in K. \tag{VIII.30}$$

To show that the ensuing map $B \mapsto p(B)$ is indeed a spectral measure, we need a strengthening of Lemma VIII.4. First, note that any bounded Borel function $f : R \to \mathbb{C}$ can be decomposed as

$$f = f_0 - f_1 + i(f_2 - f_3), \tag{VIII.31}$$

with all $f_i \geq 0$. Definition (VIII.29) then applies to each of the four terms in the decomposition of f, and we can define

$$f(a) := f_0(a) - f_1(a) + i(f_2(a) - f_3(a)). \tag{VIII.32}$$

Theorem VIII.7 *Let $a^* = a$ be a bounded operator on H. Let again $K = [-k, k] \subset \mathbb{R}$ be such that $[-\|a\|, \|a\|] \subset K$.*

1. *The map $f \mapsto f(a)$ from the space of bounded Borel functions $f : K \to \mathbb{C}$ to the bounded operators on H is an algebra homomorphism in the sense that*

$$\begin{aligned} (t_1 f + t_2 g)(a) &= t_1 f(a) + t_2 g(a); && \text{(VIII.33)} \\ (fg)(a) &= f(a)g(a); && \text{(VIII.34)} \\ \overline{f}(a) &= f(a)^*. && \text{(VIII.35)} \end{aligned}$$

   Here fg is the pointwise product of f and g and $t_i \in \mathbb{R}$.

2. *The map $f \mapsto f(a)$ preserves positivity in the sense that*

$$f(x) \leq g(x)\, \forall x \in K \;\Rightarrow\; f(a) \leq g(a). \tag{VIII.36}$$

3. *If (f_n) is a bounded monotone increasing sequence of (Borel) functions on K converging pointwise to f, then $f(a) = \lim_n f_n(a)$ (strong limit, i.e., $f(a)\psi = \lim_n f_n(a)\psi$ for each $\psi \in H$).*

4. *One has*
$$\|f(a)\| \leq \|f\|_\infty = \sup_{x\in K} |f(x)|. \tag{VIII.37}$$

To prove this, we need a new description of the strong limit a in (VIII.27). Namely, under the conditions of Lemma VIII.6 one has

$$a := \text{s-}\lim_n a_n = \sup_n a_n, \tag{VIII.38}$$

the least upper bound of the a_n under the partial ordering $\leq$ for operators. This means that a is the unique positive operator for which $a_n \leq a$ and if $a_n \leq b \leq a$, then $b = a$. Namely, $a_n\psi \to a\psi$ implies $(\psi, a_n\psi) \to (\psi, a\psi)$, hence by real analysis $(\psi, a\psi) = \sup\{(\psi, a_n\psi)\}$. If b is as above then $(\psi, a_n\psi) \leq (\psi, b\psi) \leq (\psi, a\psi)$. Taking the supremum over n then gives $(\psi, b\psi) = (\psi, a\psi)$ for all ψ. Now (exercise), it can be shown that because $b^* = b$ and $a^* = a$ this equality implies $b = a$.

This leads to an easy proof of the theorem. One splits f and g into four positive parts as above. Then (VIII.33) and (VIII.35) are easy. To prove (VIII.34), its is sufficient to show that $f^2(a) = f(a)^2$ (why?). Using Lemma VIII.5 and realizing that if $p_n \to f$ pointwise then $p_n^2 \to f^2$, this comes down to showing that

$$\text{s-}\lim_n(b_n^2) = (\text{s-}\lim_n b_n)^2, \tag{VIII.39}$$

for $b_n = p_n(a)$. But this is true in general: if (b_n) is a monotone increasing bounded sequence of bounded self-adjoint operators strongly converging to b, then, using (VIII.38) the property (VIII.39) is equivalent to

$$\sup\{b_n^2\} = b^2. \tag{VIII.40}$$

This is indeed correct: if $c := \sup\{b_n^2\}$ is the left-hand side, then by definition

$$(\psi, c\psi) = \sup\{(\psi, b_n^2\psi)\} = \sup\{\|b_n\psi\|^2\} = \lim_n \|b_n\psi\|^2 = \|\lim_n b_n\psi\|^2 = \|b\psi\|^2 = (\psi, b^2\psi).$$

This holds for all $\psi \in H$, so that $c = b^2$.

Eq. (VIII.36) follows from Lemma VIII.4. The third claim follows by approximating each f_n pointwise by polynomials; we leave the details to the reader as an exercise. The last claim will be proved at the end of the next section. ■

Corollary VIII.8 *The map $B \mapsto p(B)$ defined by* (VIII.8) *in terms of a bounded self-adjoint operator a is a spectral measure (cf. Definition VIII.1).*

Indeed, the properties 1-5 in Definition VIII.1 faithfully reflect the following properties op characteristic functions:

1. $\chi_\emptyset = 0$;
2. $\chi_{\mathbb{R}} = 1$;
3. $\chi_{A\cap B} = \chi_A\chi_B$;
4. $\chi_{A\cup B} = \chi_A + \chi_B$ when $A \cap B = \emptyset$;
5. $\chi_{\cup_n B_n} = \sup\{\chi_{B_n}\}$.

Finally, the spectral measure associated to a is related to the spectrum $\sigma(a)$ of a in the following way.

Proposition VIII.9 *One has $\lambda \in \sigma(a)$ iff $p(\lambda - \epsilon, \lambda + \epsilon) \neq 0$ for all $\epsilon > 0$.*

Write this as $A \Leftrightarrow B$. To prove the "$\Rightarrow$" direction, we prove that not$B \Rightarrow$ not$A$, i.e. that if $p(\lambda-\epsilon,\lambda+\epsilon) = 0$ for some $\epsilon > 0$, then $\lambda \in \rho(a)$. Indeed, consider $g : \mathbb{R} \to \mathbb{R}$ defined by $g(x) := (x-\lambda)^{-1}$ for $x \notin (\lambda-\epsilon,\lambda+\epsilon)$ and $g(x) := 0$ for $x \in (\lambda-\epsilon,\lambda+\epsilon)$. Then g is bounded, hence $g(a)$ is defined. In what follows, we repeatedly use part 1 of Theorem VIII.7. First, since

$$g(x)(x-\lambda)\chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(x) = \chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(x)$$

for all $x \in \mathbb{R}$, one has

$$g(a)(a-\lambda)\chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(a) = \chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(a). \tag{VIII.41}$$

However, since

$$\chi_{(\lambda-\epsilon,\lambda+\epsilon)} + \chi_{(\lambda-\epsilon,\lambda+\epsilon)^c} = 1$$

one has

$$\chi_{(\lambda-\epsilon,\lambda+\epsilon)}(a) + \chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(a) = 1. \tag{VIII.42}$$

But $\chi_{(\lambda-\epsilon,\lambda+\epsilon)}(a) = p(\lambda-\epsilon,\lambda+\epsilon) = 0$ by assumption, so that (VIII.42) yields $\chi_{(\lambda-\epsilon,\lambda+\epsilon)^c}(a) = 1$. Hence (VIII.41) reads $g(a)(a-\lambda) = 1$. Similarly, $(a-\lambda)g(a) = 1$. It follows that $g(a)$ is a bounded inverse to $a-\lambda$, so that by definition $\lambda \in \rho(a)$.

To prove $B \Rightarrow A$, we use Theorem VII.15. Assume $p(\lambda-\epsilon,\lambda+\epsilon) \neq 0$ for all $\epsilon > 0$. Take $\epsilon = 1/n$ and find a unit vector $\psi_n \in p(\lambda-1/n,\lambda+1/n)H$. Then

$$\|(a-\lambda)\psi_n\| \leq \|(a-\lambda)p(\lambda-1/n,\lambda+1/n)\| \leq 1/n; \tag{VIII.43}$$

the last estimate follows from (VIII.37), since

$$\sup_{t\in\mathbb{R}} |(t-\lambda)\chi_{(\lambda-\epsilon,\lambda+\epsilon)}(t)| = \epsilon.$$

Hence $\|(a-\lambda)\psi_n\| \to 0$, so that $\lambda \in \sigma(a)$ by Theorem VII.15. ■

Corollary VIII.10 *Let $B \mapsto p(B)$ be defined by* (VIII.8). *If $B \cap \sigma(a) = \emptyset$, then $p(B) = 0$.*

Now notice that for bounded $a = a^*$ one has $\sigma(a) \subseteq [-\|a\|,\|a\|]$. (Exercise: if $z \notin [-\|a\|,\|a\|]$, then $a-z$ is invertible, hence $z \in \rho(a)$. This follows from Lemma VII.9). Hence everything we have done so far is independent of the choice of K, as long as it is compact (so that every polynomial $p : K \to \mathbb{R}$ is bounded) and contains $[-\|a\|,\|a\|]$.

Finally, it is an interesting exercise to derive the examples (VIII.11) etc. in the previous section from the rigorous definition of the spectral measure in the present section.

VIII.3 The spectral theorem for bounded operators

The map $B \mapsto P(B)$ defined by (VIII.8) generalizes the projections p_i in the spectral theory of compact operators. We now turn to the generalization of the expansion (VIII.1). To state this, we first define a map $t \mapsto E(t)$ from $\mathbb{R}$ to the set of projections on H by

$$E(t) := p((-\infty,t]) = \text{s-}\lim_{s\to\infty} p([s,t]), \tag{VIII.44}$$

where $p(B)$ for $B \subset \mathbb{R}$ is given by (VIII.8). In other words,

$$E(t) = \chi_{(-\infty,t]}(a). \tag{VIII.45}$$

Using part 1 of Theorem VIII.7, it is easily shown that $E(t)$ is a projection, since

$$E(t)^2 = \chi_{(-\infty,t]}(a)^2 = \chi^2_{(-\infty,t]}(a) = \chi_{(-\infty,t]}(a) = E(t)$$

and

$$E(t)^* = \chi_{(-\infty,t]}(a)^* = \overline{\chi_{(-\infty,t]}}(a) = \chi_{(-\infty,t]}(a) = E(t).$$

For example, combining (VIII.7) and (VIII.44), we have, for compact $a = a^*$,

$$E(t) = \sum_{i|\lambda_i \le t} p_i. \tag{VIII.46}$$

Similarly, from (VIII.13) and (VIII.44) we obtain

$$E(t) = \chi_{a\le t} := \chi_{\{x\in\mathbb{R}^n | a(x)\le t\}}. \tag{VIII.47}$$

The map $t \mapsto E(t)$ defines a so-called **spectral density** in the sense that the following properties hold.

1. E is monotone increasing, that is, $E(s) \le E(t)$ if $s \le t$. For projections, this is equivalent to $E(s)H \subseteq E(t)H$.
2. E is strongly *right*-continuous, that is, s-$\lim_{\varepsilon\to 0^+} E(t+\varepsilon) = E(t)$.
3. s-$\lim_{t\to-\infty} E(t) = 0$ and s-$\lim_{t\to\infty} E(t) = 1$.

The first property follows from (VIII.36). The others follow from the third claim in Theorem (VIII.7) and the corresponding pointwise limits of $\chi_{(-\infty,t]}$, e.g., $\lim_{t\to-\infty} \chi_{(-\infty,t]}(x) = 0$ for all $x \in \mathbb{R}$.

The spectral theorem now has the following form.

Theorem VIII.11 *Let a be a bounded self-adjoint operator on H and let $f : \mathbb{R} \to \mathbb{R}$ be a bounded (Borel) function. Then*

$$f(a) = \int dE(t)\, f(t). \tag{VIII.48}$$

In particular, the cases $f(t) = t$ and $f(t) = 1$ generalize (VIII.1) and (VIII.3), respectively:

$$a = \int dE(t)\, t; \tag{VIII.49}$$

$$1 = \int dE(t). \tag{VIII.50}$$

To make sense of this theorem, we need to define the integral. As we shall see, defining it already proves the theorem. We proceed in four steps.

1. For $f = \chi_B$ we put
$$\int dE(t)\, \chi_B(t) := p(B) = \chi_B(a). \tag{VIII.51}$$
2. For a simple function $f = \sum_k c_k \chi_{B_k}$ (finite sum) with $c_k \ge 0$ we define the integral by extending the previous case by linearity, i.e.
$$\int dE(t) \sum_k c_k \chi_{B_k} := \sum_k c_k p(B_k) = \sum_k c_k \chi_{B_k}(a). \tag{VIII.52}$$
This already proves the spectral theorem for simple functions, since if f is simple, then (VIII.52) coincides with (VIII.49).
3. For general bounded positive (Borel) functions f, we use Lemma VIII.12 to find a sequence (s_n) of simple functions (subject to the conditions stated in the lemma) converging pointwise to f to define
$$\int dE(t)\, f(t) \equiv \int dE(t)\, \lim_n s_n(t) := \text{s-}\lim_n \int dE(t)\, s_n(t). \tag{VIII.53}$$
By (VIII.52), this equals
$$\int dE(t)\, f(t) = \text{s-}\lim_n s_n(a). \tag{VIII.54}$$
The existence of this limit follows in the same way as in (VIII.29), with polynomials replaced by simple functions.

4. Finally, the general (i.e. complex) case follows as in (VIII.31) and defining the integral by linearity, i.e. if $f = f_0 - f_1 + i(f_2 - f_3)$ with all $f_i \geq 0$, then

$$\int dE(t)\, f(t) := \int dE(t)\, f_0(t) - \int dE(t)\, f_1(t) + i(\int dE(t)\, f_2(t) - \int dE(t)\, f_3(t)). \quad \text{(VIII.55)}$$

If we now use the the third claim in Theorem (VIII.7), we see that the right-hand side of (VIII.54) is just $f(a)$. This proves Theorem VIII.11. ■

As we have seen, proving the spectral theorem is just a matter of defining the integral in the right way! The only substantial result on which the proof relies is this:

Lemma VIII.12 *Let $K = [-k, k] \subset \mathbb{R}$, $k \in \mathbb{R}^+$. For each positive bounded (Borel) function $f : K \to \mathbb{R}$ there exists a bounded monotone increasing sequence (s_n) of simple functions on K that converges pointwise to f.*

We still owe the reader a proof of part 4 of Theorem VIII.7. As easily follows from the definition, one may estimate the norm of the integral (VIII.48) using the familiar rules, like

$$\|f(a)\| = \| \int dE(t)\, f(t)\| \leq \| \int dE(t)\| \|f\|_\infty = \|f\|_\infty, \quad \text{(VIII.56)}$$

where we have used (VIII.50).

Finally, to recognize (VIII.1) as a special case of (VIII.49), we need the following result (cf. Prop. VIII.9).[3]

Proposition VIII.13 *One has $\lambda \in \sigma_d(a)$ iff $p(\{\lambda\}) \neq 0$, in which case $p(\{\lambda\})$ equals the projection onto the eigenspace H_λ of a.*

To prove this, we write $p(\lambda) \equiv p(\{\lambda\})$ and denote the projection onto the eigenspace H_λ by p_λ (provided $\lambda \in \sigma_d(a)$). We have $p(\lambda) = \chi_\lambda(a)$ by (VIII.8); we write $\chi_\lambda \equiv \chi_{\{\lambda\}}$. Hence

$$ap(\lambda) = \mathrm{id}(a)\chi_\lambda(a) = (\mathrm{id} \cdot \chi_\lambda)(a) = (\lambda 1 \chi_\lambda)(a) = \lambda 1(a)\chi_\lambda)(a) = \lambda p(\lambda).$$

Consequently, if $p(\lambda) \neq 0$ then $p_\lambda \neq 0$, so that $\lambda \in \sigma_d(a)$, and

$$p(\lambda) \leq p_\lambda, \quad \text{(VIII.57)}$$

since $p(\lambda)H \subseteq p_\lambda H = H_\lambda$, as we have just shown.

Conversely, let $f_n(t) := (\inf\{1, |\lambda - t|\})^{1/n}$, so that $f_n \to \chi_{\mathbb{R}\setminus\{\lambda\}}$ pointwise. Hence by Theorem VIII.7 (part 3) one has $f_n(a) \to \chi_{\mathbb{R}\setminus\{\lambda\}}(a) = p(\mathbb{R}\setminus\{\lambda\})$. Now, if $\lambda \in \sigma_d(a)$, so that $p_\lambda \neq 0$, then

$$f_n(a)p_\lambda f = f_n(\lambda)p_\lambda f = 0 \quad \text{(VIII.58)}$$

for all $f \in H$; for in general one has $f(a)p_\lambda f = f(\lambda)p_\lambda$, as can be seen by approximating f by polynomials (for which the property is clearly true) and using Theorem VIII.7. Letting $n \to \infty$ in (VIII.58) yields $p(\mathbb{R}\setminus\{\lambda\})p_\lambda = 0$, or $p(\lambda)p_\lambda = p_\lambda$, as $p(\mathbb{R}\setminus\{\lambda\}) + p(\lambda) = 1$. In other words,

$$p(\lambda) \geq p_\lambda. \quad \text{(VIII.59)}$$

With (VIII.57), we obtain $p(\lambda) = p_\lambda$. ■

Consequently, if $\sigma(a) = \sigma_d(a)$ the integral in (VIII.49) only picks up contributions from $t = \lambda_i \in \sigma_d(a)$. Approximating the function $f(t) = t$ in the appropriate way then yields (VIII.1) (exercise).

[3] Recall that the discrete spectrum $\sigma_d(a)$ consists of all eigenvalues of a.

VIII.4 The spectral theorem for unbounded operators

The spectral Theorem VIII.11 is valid when a and f are bounded. If both are possibly unbounded, the claim is as follows.

Theorem VIII.14 *Let $a : D(a) \to H$ be a self-adjoint operator on and let $f : \mathbb{R} \to \mathbb{R}$ be a (Borel) function. Then*

$$f(a) = \int dE(t)\, f(t) \tag{VIII.60}$$

is self-adjoint on

$$D(f(a)) = \{\psi \in H \mid \int dP_\psi(t)\, |f(t)|^2 < \infty\}. \tag{VIII.61}$$

In particular,

$$a = \int dE(t)\, t \tag{VIII.62}$$

and

$$D(a) = \{\psi \in H \mid \int dP_\psi(t)\, t^2 < \infty\}. \tag{VIII.63}$$

Recall that the probability measure P_ψ is given by (VIII.20). Integrals of the type $\int dP_\psi(t)\, f(t)$ are defined as follows (cf. the proof of Theorem VIII.11): start with $\int dP_\psi(t)\, \chi_B(t) := P_\psi(B)$, extend this to simple functions by linearity and for positive f define

$$\int dP_\psi(t)\, f(t) = \int dP_\psi(t)\, \lim_n s_n(t) := \lim_n \int dP_\psi(t)\, s_n(t), \tag{VIII.64}$$

where s_n are simple functions and $\lim_n s_n = f$ pointwise. Finally, extend to arbitrary f using (VIII.31) and linearity.

We are going to prove Theorem VIII.14 using a method due to von Neumann [15], which derives the spectral theorem for unbounded self-adjoint operators from the spectral theorem for unitary operators. We omit the proof of (VIII.61).

Theorem VIII.15 *Let u be a unitary operator on H. Then there exists a unique spectral density E on H with the properties $E(0) = 0$ (hence $E(t) = 0$ for all $t \leq 0$), $E(2\pi) = 1$ (hence $E(t) = 1$ for all $t \geq 2\pi$), and*

$$u = \int_0^{2\pi} dE(t)\, e^{it}. \tag{VIII.65}$$

Furthermore, for bounded measurable functions $f : \mathbb{T} \to \mathbb{C}$ (where $\mathbb{T}$ is the unit circle in $\mathbb{C}$) one has

$$f(u) = \int_0^{2\pi} dE(t)\, f(e^{it}). \tag{VIII.66}$$

The proof is practically the same as for self-adjoint operators, with the following difference. In the self-adjoint case we started with polynomials p in a real variable t, defined $p(a)$ in the obvious way, and subsequently defined $f(a)$ for arbitrary bounded (Borel) functions f by approximating the latter by polynomials. The properties $p(a)^* = \overline{p}(a)$ and $p(a) \leq q(a)$ if $p(t) \leq q(t)$ for all (relevant) t then implied the corresponding properties for arbitrary f (see Theorem VIII.7). These properties hold by virtue of the equality $a^* = a$. Now, for unitary operators u one instead has

$$u^*u = uu^* = 1. \tag{VIII.67}$$

Reflecting this change, we now start from polynomials in the variable $\exp(it)$, so that the map $f \mapsto f(u)$ is initially defined for functions of the form $f(\exp it) = \sum_k c_k \exp(itk)$, which is mapped to $f(u) := \sum_k c_k u^k$. Here we may assume that $0 < t \leq 2\pi$. From this point onwards, the proof of the spectral theorem is the same as in the self-adjoint case. ∎

To prove Theorem VIII.14 from Theorem VIII.15, von Neumann introduced an operator version of the **Cayley transform**. For numbers, this is a map $\kappa : \mathbb{R} \to \mathbb{C}$ defined by

$$\kappa(t) := \frac{t-i}{t+i}. \tag{VIII.68}$$

This maps $\mathbb{R}$ homeomorphically (that is, continuously and bijectively with continuous inverse) to $\mathbb{T}\backslash\{1\}$ (i.e., the unit circle in the complex plane minus the point 1). Moreover, since formally $\kappa(-\infty) = \kappa(\infty) = 1$, it maps the one-point compactification $\dot{\mathbb{R}}$ homeomorphically to $\mathbb{T}$. The inverse is

$$\kappa^{-1}(z) = i\frac{1+z}{1-z}, \tag{VIII.69}$$

where $z \in \mathbb{T}\backslash\{1\}$. Now let a be a self-adjoint operator. We see from Theorem VII.12 that $-i \in \rho(a)$, so that $a + i : D(a) \to H$ is a bijection with bounded inverse $(a+i)^{-1} : H \to D(a)$. Composing with $a - i : D(a) \to H$, which is a bijection, too, we see that

$$\kappa(a) := \frac{a-i}{a+i} = (a-i)(a+i)^{-1} \tag{VIII.70}$$

is a bijection from H to H. In a diagram, we have

$$H \overset{(a+i)^{-1}}{\longrightarrow} D(a) \overset{a-i}{\longrightarrow} H.$$

Furthermore, since $a^* = a$ one computes $\|(a+i)\psi\| = \|(a-i)\psi\|$ for all $\psi \in D(a)$, and putting $\psi = (a+i)^{-1}\varphi$ we find $\|\varphi\| = \|\kappa(a)\|$. In other words, $\kappa(a)$ is an isometry, and since an invertible isometry is unitary, we conclude that $\kappa(a)$ *is unitary*. We note that

$$R(1 - \kappa(a)) = D(a), \tag{VIII.71}$$

since $1 - \kappa(a) = 2i(a+i)^{-1}$, and as we have seen $(a+i)^{-1} : H \to D(a)$ is a bijection.

Conversely, let u be a unitary operator with $R(1-u)^- = H$. (For example, $u = 1$ does *not* satisfy this assumption!) It is an easy exercise to show that this implies that $1 - u$ is injective, so that $1 - u : H \to R(1-u)$ is invertible. We may then define an operator on the dense domain $D(\kappa^{-1}(u)) := R(1-u)$ by

$$\kappa^{-1}(u) := i\frac{1+u}{1-u} = i(1+u)(1-u)^{-1}. \tag{VIII.72}$$

If $u = \kappa(a)$ then clearly $\kappa^{-1}(u) = a$ (including its domain), justifying the notation κ^{-1}. Consequently:

Proposition VIII.16 *The operator Cayley transform $a \mapsto \kappa(a)$ establishes a bijection between the class of self-adjoint operators a and the class of unitary operators u with $R(1-u)^- = H$.*

Now let $u = \kappa(a)$ and put

$$f(e^{it}) = \kappa^{-1}(\exp(it)) \tag{VIII.73}$$

in (VIII.66); this yields $f(u) = \kappa^{-1}(u) = a$, so that

$$a = i\int_0^{2\pi} dE(t)\, \frac{1+e^{it}}{1-e^{it}}. \tag{VIII.74}$$

A chnage of variables $t \mapsto \lambda$, where $\lambda(t) := \kappa^{-1}(\exp(it))$ gives

$$a = \int_{\mathbb{R}} d\tilde{E}(\lambda)\, \lambda, \tag{VIII.75}$$

where $\tilde{E}(\lambda) := E(t(\lambda))$, where $t(\lambda)$ is the unique $t \in (0, 2\pi]$ for which $\kappa(\lambda) = \exp(it)$. With a change of notation, this is precisely (VIII.65), up to the domain. The argument for $f(a)$ is similar, starting from (VIII.66). ∎

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